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CONTROL OF BATCH REACTIONS WITH
UNCERTAIN PARAMETERS

BY



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A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH
IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE
OF MASTER OF SCIENCE

DEPARTMENT OF CHEMICAL AND PETROLEUM ENGINEERING

EDMONTON, ALBERTA

SPRING, 1972

UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance a thesis entitled CONTROL OF BATCH REACTIONS WITH UNCERTAIN PARAMETERS submitted by Liang-Juh Lai in partial fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

ABSTRACT

This thesis is concerned with the control of batch reactions which contain uncertain parameters. Simulation results are presented for two reaction systems, a single reversible reaction and the complex reaction system of Rosenbrock and Storey [10].

Optimal and suboptimal control policies were studied and compared under ideal conditions of noise free measurements and known kinetic parameters. The suboptimal control policies resulted in a final yield close to the values for the optimal control policy. The parameter sensitivity of optimal and suboptimal control policies was also investigated to determine the feasibility of the various control policies when parameters are changed in an unanticipated manner.

To cope with the problem of unknown parameters or undetected parameter variations, a nonlinear filter technique was used to perform on-line parameter estimation. To reduce the computational requirements associated with on-line parameter estimation, two simplified nonlinear filter algorithms were also investigated. It was found that the simplified algorithms provide a feasible approach for parameter estimation and resulted in significant reduction in computation time. However, the initial covariance matrix $\underline{P}(0)$ must usually be determined by trial and error.

The robustness of the proposed nonlinear filter algorithms was verified by investigating the effect of data sampling interval, noise level and inaccurate initial estimates of states. The simplified filter

algorithms were at least as robust as the original filter.

The use of a nonlinear filter in the feedback control resulted in improved control when the kinetic parameters changed and were "tracked" by the filter.

ACKNOWLEDGEMENTS

The author is greatly indebted to his supervisor, Dr. D. E. Seborg, for his most helpful guidance, suggestions and assistance.

Grateful acknowledgements are also due to:

- (1) Department of Chemical and Petroleum Engineering for providing teaching assistantships.
- (2) National Research Council of Canada for some financial support as well as a grant for supplying the necessary computer time.
- (3) Dr. Chuang and Mr. Hong for assistance in preparing this thesis.
- (4) The staff of the Department of Computer Sciences for assistance in improving the computer program.
- (5) Mrs. Betty Boon for typing this thesis.

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CHAPTER I

INTRODUCTION

Although continuous operation offers many well-known advantages, many industrial processes are still run on a batch basis. Conditions which favor batch operation include low volume, multiple step processing, low rates of reaction, and the desire for flexibility when product obsolescence is of concern [1]. In the chemical industry, batch reactors are widely used in the manufacture of fine chemicals, pharmaceuticals and polymers.

The control and automation problems associated with batch reactors differ significantly from those of continuous reactors in several ways [2]:

- (1) Batch operation is inherently unsteady state with reactor conditions changing over a wide range of values. Reactor start up is a daily routine rather than an infrequent occurrence, as in continuous processes.
- (2) A batch process typically consists of a series of sequential steps with relatively large labor requirements. Consequently, automation will require a logical sequencing system and a digital computer is an obvious candidate if the necessary economic justification can be made.
- (3) Physical and analytical measurements are much more difficult to obtain in batch processes. Because

reactor conditions vary widely during batch operation, the measurement range is large and yet accuracy requirements for measurements are higher in batch processes. By contrast, for a well-tuned continuous process inaccurate measurements can be tolerated as long as a reasonable degree of reproducibility is attained [1].

For continuous processes, well-known control system design techniques can be employed providing that a satisfactory linear (or linearized) process model is available. In particular, single-variable feedback control systems based on transfer function process models have been widely used in the process industries. However, for batch reactors the inherently nonlinear chemical kinetics and wide range of reactor operating conditions discourage the use of a linear process model such as a transfer function.

An important consideration in designing a batch reactor control system is the sensitivity of the control system performance to the assumed values of the process parameters. Reaction rate expressions which are accurate over a wide range of conditions are very difficult to determine. Furthermore, for batch reactors, the characteristics of the initial charge may change unpredictably from batch to batch due to variations in feed composition, catalyst properties, or improper cleaning of the reactor after the previous cycle of operation. The central concern of this study is to determine a feasible control policy for batch reactors when process parameters change unpredictably from batch to batch.

The optimal control of chemical reactors has been studied extensively during the last decade with definitive contributions being made by Aris and coworkers [3,4,5,6,7,8,9]. In this approach the objective is to determine the control policy which will maximize (or minimize) a specific "performance index". Thus a dynamic optimization problem is formulated and the solution obtained by utilization of optimization techniques such as dynamic programming, Pontryagin's maximum principle, or hill-climbing techniques [10]. For batch reactors an obvious performance index is the minimum time required to achieve a certain product yield or equivalently [3,11], the maximum yield which can be obtained in a specific time interval.

However, optimal control policies for batch reactors contain several disadvantages. Except for special cases such as a single reversible reaction, the optimal control law is typically "open loop" in that the manipulated variables are specified as a function of time rather than as a function of the measured process variables, as in a feedback control law. Consequently, process disturbances or unanticipated changes in process parameters may have a detrimental effect on control system performance. As noted above, for batch reactions parameter values may be uncertain or change unpredictably from batch to batch. Even if process parameters could be estimated "on-line" (as proposed below), updating the optimal control policy based on current parameter values is not attractive on account of the extensive calculations required to determine the optimal control policy for a nonlinear system. Such calculations would not be practical for most process control computers.

Alternatively, several "suboptimal" control schemes incorporating feedback control action have been proposed for batch reactors [12,13,14,15]. Millman and Katz [13] have studied the conventional three mode controller (proportional-integral-derivative) for several types of simulated consecutive and parallel reaction systems. Their examples indicated that the use of controller constants determined by hill-climbing techniques resulted in reaction yields which were very close to the optimal yields. However, their suboptimal control policy would also be difficult to adapt on-line to accomodate changing conditions because the required calculations are quite extensive.

A second class of suboptimal control policies for nonlinear systems is concerned with minimizing a performance index based on instantaneous process conditions rather than the process conditions during the entire time period. The resulting control scheme usually includes feedback action and can easily be updated if process parameter changes are detected by some method of parameter estimation. Suboptimal control schemes based on minimizing an instantaneous performance index have been investigated by Seinfeld both for continuous reactors [16] and batch reactors [11].

In this study the problem of interest is the determination of control policies for batch reactors whose process parameters change in an unpredictable fashion from batch to batch. The general approach adopted is to assume a process model of a particular form and estimate model parameters on-line from noisy measurements using sequential estimation techniques (i.e. nonlinear filtering). The

updated parameter estimates are continuously incorporated into the control law and thus estimation and control proceed simultaneously. This approach is often referred to as an adaptive control scheme [5,6,7,8]. A significant advantage of this approach is that estimates of inaccessible state variables such as chemical composition are automatically generated during parameter estimation. This permits the employment of "inferential control" techniques which use estimated values of unmeasured state variables for control. Such techniques have been successfully implemented by Fisher and Jacobson [17] for a pilot plant evaporator.

A major disadvantage of the proposed approach (i.e. on-line parameter estimation plus control) is that implementation will inevitably require the availability of a process control computer. However, successful industrial applications of computer control techniques for batch reactors have recently been reported [2,18,19,20]. The main justification for computer control of batch processes is the resulting reduced labor costs and improved productivity [1]. Other advantages include improved process reproducibility and precise documentation [21].

The remainder of this thesis is organized as follows. Chapter II presents a discussion of existing nonlinear filtering techniques with emphasis on simplified filters with reduced computational requirements. The combined parameter estimation and control scheme is applied to a single reaction system in Chapter III and to a complex reaction system in Chapter IV. The parameter sensitivity of both

optimal and suboptimal control schemes is investigated and the robustness of the proposed scheme to noise level, data sampling intervals and other parameters is also considered. Finally, the conclusions of this study are presented in Chapter V.

CHAPTER II

NONLINEAR FILTERING TECHNIQUES2.1 Introduction

Mathematical models of batch reactors typically consist of material and energy balances written in the form of a set of nonlinear ordinary differential equations. These models are far from precise due to the uncertainty associated with the values of process parameters such as rate constants and heat transfer coefficients, and variations in the characteristics of the initial charge from batch to batch. In this analysis it will be assumed that the effects of such modelling errors can be significantly reduced by considering certain parameters in the set of ordinary differential equations to be "unknown". The task of the adaptive control scheme is then to estimate the unknown parameters from noisy process measurements during a batch run, and to make the appropriate corrections in control action to compensate for changes in process parameters.

The general problem of estimating parameters in ordinary differential equations from noisy data has received considerable attention in recent years as indicated by the large number of articles [22,23,24,25,26], review papers [27,28,29] and books [10, 30,31,32,33,34,35] concerned with this topic.

Parameter estimation techniques can be conveniently classified as being either sequential or nonsequential methods. The characteristic feature of nonsequential estimation is that a string of input/output data is collected before the parameter estimation

begins. By contrast, in sequential estimation a parameter estimate can be generated at each sampling instant. Consequently, sequential estimation methods are well-suited for adaptive control applications where process parameters change and are to be "tracked" (i.e. estimated on-line). In addition, sequential estimation can provide estimates of state variables which are needed for control but often cannot be measured. In this thesis, state variables which are impractical or inconvenient to measure will be referred to as "inaccessible state variables".

Sequential estimation of states and parameters is often referred to as a filtering problem [29]. For nonlinear estimation, there exist several nonlinear filter techniques, such as the extended Kalman filter [32,34], Detchmendy and Sridhar filter [22], Cox filter [25,32] and many minimal variance filters [25,32]. These methods can be used for filtering out noise contained in the process and measurements, and estimating unknown parameters and inaccessible state variables. The differences between these nonlinear filter techniques lie in the different estimation criteria that are used and the approximations that are involved [35,19,30,31,32]. Since no general solution of the filtering problem is available, all of the nonlinear filter techniques require approximations to be made which introduce some degree of suboptimality.

Lately, nonlinear filter schemes have been considered in chemical engineering problems. Wells [36] used the extended Kalman filter to perform state and parameter estimation for a simulated single reaction taking place in a continuous stirred tank reactor

(CSTR). Gavallas and Seinfeld [37] used a Cox filter to estimate catalyst decay rates for a single irreversible reaction taking place isothermally in a plug flow reactor. The extended Kalman filter has been used by Seinfeld [16] to investigate the stochastic features of a single CSTR reaction. A single CSTR control scheme with time delay in the feedback control loop has also been studied [38] using a Detchmندی and Sridhar nonlinear filter to estimate the unknown kinetic parameter of a single reaction. In a batch reactor application, Lee [30] used a Detchmندی and Sridhar nonlinear filter to estimate the unknown rate constant of a single isothermal reaction. Pell [39] used a different nonlinear filter to estimate the unknown kinetic parameters of a simple consecutive reaction for both isothermal and nonisothermal conditions. Coggan and Noton [40] have used the extended Kalman filter to investigate the filter performance by simulating a complicated blending process and a thermal system. Applications of the proposed filtering schemes to physical systems of interest to chemical engineers have seldom been reported. A noteworthy exception is the application of the extended Kalman filter to an industrial reactor system [41]. However, few details of this application are available.

With so many nonlinear filters available in the literature and since different filters have been applied successfully in different examples, comparisons of different filters have also been made [23,25,32]. Wishner et al [23] compared the performance of the extended Kalman filter, a second order nonlinear filter and a single stage iteration filter, which have the same theoretical basis but are

successively more complex to implement. From their simulated results for three numerical examples, they concluded that the performance of the filter is successively improved by the additional complexity. Schwartz and Stear [25] compared the performance of eight different filters, one linear and seven nonlinear, on two scalar nonlinear systems. They concluded that none of the eight filters provided a clearcut superiority over the others. Jazwinski [32] later criticized their conclusions on the ground that the large noise levels in the Schwartz and Stear's examples masked the nonlinearity of the measurement equation; hence, the simulated filters in their examples cannot be recommended on the basis of superior performance. However, he then concluded that the relative value of different nonlinear filters in a particular problem cannot be assessed a priori, but must be determined by simulation.

In this thesis, the Detchmendy and Sridhar nonlinear filter [22] will be applied to two batch reactor examples. Since their filter is based on a weighted least square performance index, no prior statistical information about the process noise is required. However, the weighting matrices used in the performance index must be specified.

2.2 Summary of Detchmendy and Sridhar Filter^[22] Algorithm

In this section, Detchmendy and Sridhar's filter algorithm [22] is briefly described. A more detailed derivation is presented in Appendix A.

Consider a nonlinear system governed by the ordinary vector

differential equation

$$\dot{\underline{z}}(t) = \underline{g}[\underline{z}(t), \underline{p}, t] \quad (2-1)$$

where $\underline{z}$ and $\underline{p}$ are vectors of state variables and time invariant parameters, respectively, and t denotes time. Define

$$\underline{x} \equiv \begin{bmatrix} \underline{z} \\ \underline{p} \end{bmatrix} \quad (2-2)$$

then Equation (2-1) can be rewritten as

$$\dot{\underline{x}} = \begin{bmatrix} \dot{\underline{z}} \\ \dot{\underline{p}} \end{bmatrix} = \begin{bmatrix} \underline{g} \\ \underline{0} \end{bmatrix} \equiv \underline{f} \quad (2-3)$$

or

$$\dot{\underline{x}} = \underline{f}[\underline{x}(t), t] \quad (2-4)$$

Let the total dimension of $\underline{z}$ and $\underline{p}$ be n , then $\underline{x}$ becomes a n -dimensional vector and $\underline{f}(\underline{x}, t)$ is a n -dimension vector function.

In general for physical systems, dynamic errors (e.g. random noise, modelling errors) are often involved in the process. Let the dynamic error present in the process be represented by an additive term in the vector differential equation. Then the dynamic model of the process can be expressed by

$$\dot{\underline{x}}(t) = \underline{f}(\underline{x}, t) + \underline{K}(\underline{x}, t) \underline{w}(t) \quad (2-5)$$

and let the observation model also contain additive noise, $\underline{v}(t)$, with

$$\underline{y}(t) = \underline{h}(\underline{x}, t) + \underline{v}(t) \quad (2-6)$$

where

$\underline{y}(t)$ = m-vector of outputs (i.e. measured variables)

$\underline{K}(\underline{x}, t)$ = $n \times l$ matrix,

$\underline{h}(\underline{x}, t)$ = m-vector function

$\underline{w}(t)$ = l -vector of unknown

$\underline{v}(t)$ = m-vector of measurement

inputs ,

errors

with $\underline{w}(t)$ and $\underline{v}(t)$ assumed to be random variables with unknown statistics.

By measuring $\underline{y}(t)$, it is desired to find the least squares estimate of $\underline{x}(t)$, denoted by $\hat{\underline{x}}(t)$, such that the following performance index is minimized.

$$I = \int_0^{t_f} [\|\underline{y}(t) - \underline{h}(\hat{\underline{x}}, t)\|_{\underline{Q}(t)}^2 + \|\dot{\hat{\underline{x}}} - \underline{f}(\hat{\underline{x}}, t)\|_{\underline{W}(t)}^2] dt \quad (2-7)$$

where t_f is the specified final time and $\underline{Q}(t)$ and $\underline{W}(t)$ are weighting matrices which determine the relative weighting to be placed on the individual terms in the performance index.

By applying Pontryagin's maximum principle to the dynamic optimization problem posed by Equations (2-4)-(2-7), and making certain approximations (see Appendix A), Detchmندی and Sridhar [22] derived the following filter

$$\dot{\hat{\underline{x}}}(t) = \underline{f}(\underline{x}, t) + \underline{P}(t) \left[\frac{\partial \underline{h}'(\hat{\underline{x}}, t)}{\partial \hat{\underline{x}}} \right] \underline{Q}(t) [\underline{y}(t) - \underline{h}(\hat{\underline{x}}, t)] \quad (2-8)$$

The first part of the paper is devoted to the study of the

properties of the function $f(x)$ defined by the equation

$$f(x) = \int_0^x \frac{1}{1+t^2} dt, \quad (1)$$

where x is a real number. It is well known that

$$f(x) = \arctan x, \quad (2)$$

and that the function $f(x)$ is continuous and differentiable

for all real values of x . The function $f(x)$ is also

bounded for all real values of x , and its range is the

interval $(-\pi/2, \pi/2)$. The function $f(x)$ is also

odd, and its graph is a curve passing through the origin

and having a horizontal asymptote at $y = \pi/2$.

The function $f(x)$ is also concave down for all real

values of x , and its graph is a curve that is

increasing and concave down for all real values of x .

The function $f(x)$ is also a solution of the differential

$$f'(x) = \frac{1}{1+x^2}, \quad (3)$$

with the initial condition $f(0) = 0$. The function $f(x)$

is also a solution of the differential equation

$$f''(x) = -\frac{2x}{1+x^2}, \quad (4)$$

with the initial condition $f'(0) = 1$. The function $f(x)$

$$\begin{aligned}
\dot{\underline{\underline{P}}}(t) = & \left[\frac{\partial \underline{\underline{f}}(\hat{\underline{x}}, t)}{\partial \hat{\underline{x}}} \right] \underline{\underline{P}}(t) + \underline{\underline{P}}(t) \left[\frac{\partial \underline{\underline{f}}'(\hat{\underline{x}}, t)}{\partial \hat{\underline{x}}} \right] \\
& + \underline{\underline{P}}(t) \frac{\partial}{\partial \hat{\underline{x}}} \left[\left(\frac{\partial \underline{\underline{h}}'(\hat{\underline{x}}, t)}{\partial \hat{\underline{x}}} \right) \underline{\underline{Q}}(t) (\underline{y}(t) - \underline{\underline{h}}(\hat{\underline{x}}, t)) \right] \underline{\underline{P}}(t) \\
& + \underline{\underline{K}}(\hat{\underline{x}}, t) \underline{\underline{V}}^{-1}(\hat{\underline{x}}, t) \underline{\underline{K}}'(\hat{\underline{x}}, t)
\end{aligned} \tag{2-9}$$

with

$$\underline{\underline{V}}(\hat{\underline{x}}, t) = \underline{\underline{K}}'(\hat{\underline{x}}, t) \underline{\underline{W}}(t) \underline{\underline{K}}(\hat{\underline{x}}, t) \tag{2-10}$$

where $\underline{\underline{h}}'(\hat{\underline{x}}, t)$ and $\underline{\underline{K}}'(\hat{\underline{x}}, t)$ are the corresponding transposes of $\underline{\underline{h}}(\hat{\underline{x}}, t)$ and $\underline{\underline{K}}(\hat{\underline{x}}, t)$, $\underline{\underline{V}}^{-1}(\hat{\underline{x}}, t)$ is the inverse of $\underline{\underline{V}}(\hat{\underline{x}}, t)$ and $\underline{\underline{P}}(t)$ is an $n \times n$ symmetric matrix which can be roughly interpreted as the covariance of the random vector $\hat{\underline{x}}(t)$ [37]. Integration of Equations (2-8) and (2-9) provides an estimate $\hat{\underline{x}}(t)$ of the actual state $\underline{x}(t)$ based on measurements of the output, $\underline{y}(t)$.

In this filter estimation, $\hat{\underline{x}}$ and $\underline{\underline{P}}$ are always coupled and evaluated simultaneously after specifying the initial values of $\underline{\underline{Q}}(0)$, $\underline{\underline{W}}(0)$, $\underline{\underline{P}}(0)$ and $\hat{\underline{x}}(0)$ and choosing a final time t_f . Hence the total number of differential equations that are investigated during filtering becomes $n + n(n + 1)/2 = n(n + 3)/2$. By analogy with the Kalman filter which is optimal for a linear system, the weighting matrices, $\underline{\underline{Q}}(t)$ and $\underline{\underline{W}}(t)$, can be chosen as the inverse of the covariance matrices of the output measurement error, $\underline{v}(t)$, and input noise, $\underline{\underline{K}}(\underline{x}, t)\underline{w}(t)$, respectively [31]. Similarly, for the Kalman filter, $\underline{\underline{P}}(0)$ is chosen to be the inverse of the covariance matrix for the initial state, $\underline{x}(0)$, assuming it is a random variable with

unknown statistics [31,37]. Since approximations are used in deriving the filter equations, the initial value of $\underline{\underline{p}}(0)$ is not known exactly; hence numerical experimentation is usually required to find a satisfactory value [31].

2.3 Simplified Filter Algorithm - I

In using Detchmندی and Sridhar's nonlinear filter, $\frac{n(n+3)}{2}$ differential equations must be integrated to determine n state variables (including the unknown parameters). Since the estimation of $\hat{\underline{x}}$ and $\underline{\underline{p}}$ are always coupled and solved simultaneously at each sampling instance, the filter estimation, which requires matrix manipulation and integration, becomes very time consuming when n is large. However, in most industrial situations, the digital computer used for real-time applications is a small or medium size computer, such as the IBM 1800, with restrictions on memory size and execution speed. Thus the computation time of filter estimation becomes a severe point for real-time applications.

For the extended Kalman filter, Dressler and Ross [42] have stated that they investigated several approximate filter algorithms in order to reduce the computation time without significantly degrading the filter performance. They found the most promising simplified filter algorithm to be one which uses a piecewise recursive estimation [42]. The basic idea of the proposed piecewise recursive estimation scheme is to separate the filter estimation into two estimation "loops"; one for state estimation and one for the covariance equations. This can be explained as follows.

In a typical filtering application, the state estimate $\hat{\underline{x}}(t)$ and the covariance matrix $\underline{P}(t)$ are generated by numerical integration using the data sampling interval, t_s , as the integration interval. Thus a sequence of values, $\hat{\underline{x}}(nt_s)$ and $\underline{P}(nt_s)$, are generated for $n = 0, 1, 2, \dots$. Dressler and Ross [42] proposed that the covariance equations be updated every M sampling intervals where M is an integer greater than one. This strategy will result in a significant reduction in the computational requirements for the filter. It also has the effect of maintaining $\underline{P}(t)$ constant over M sampling interval while $\hat{\underline{x}}$ is still updated every sampling interval. In effect $\underline{P}(t)$ becomes piecewise constant and the amount of computations required to integrate the covariance equations is reduced by a factor of M .

Dressler and Ross [42] have applied their "piecewise recursive" modification of the extended Kalman filter to a simple second order numerical example. Apparently, this is the only published application of this approach. In this study, the piecewise recursive modification will be further evaluated as a modification to the Detchmندی and Sridhar filter and by application of the resulting filter to two batch reactor examples.

2.4 Simplified Filter Algorithm - II

A second type of simplified nonlinear filter technique has been proposed by Seinfeld and Chen [14]. The basic idea is to replace the covariance differential equations by algebraic expressions for the elements of $\underline{P}(t)$. Since the computation time required to integrate differential equations will, in general, be much greater than

that for evaluating simple algebraic expressions, the reduction in computational time and storage requirements can be very significant for real time applications. A systematic method for determining the algebraic expressions is to examine the time behavior of $\underline{\underline{P}}(t)$ during estimation using the original filter. Then the response of the elements of $\underline{\underline{P}}(t)$ can be roughly approximated by the use of simple functions such as exponentials [14].

The only known application of this technique is the reactor example in the unpublished work by Seinfeld and Chen [14]. Hence further evaluation of this approach would appear to be desirable.

CHAPTER III

STUDIES OF A SINGLE REACTION

3.1 Formulation

The optimal temperature control for a chemical reaction occurring in a batch reactor has two equivalent senses: it will achieve the maximum yield in a fixed time and it will require the minimum amount of time to achieve a certain conversion. For a single reaction, only reversible exothermic reactions provide interesting optimization and control problems. By contrast, in endothermic reactions heat is absorbed and the optimal control policy is to provide as much heat as is possible. For a single exothermic reaction the optimal temperature control policy is to maximize the reaction rate at each instant of time [3,11]. It has been found that the optimal temperature of a single reversible exothermic reaction is somewhat less than the equilibrium temperature at any given composition [3,11].

Consider a single reversible exothermic reaction taking place in a constant volume batch reactor. If the chemical species present are $A_1, A_2, \dots, A_S$ the reaction stoichiometry can be written as [3]

$$\sum_{i=1}^S \alpha_i A_i = 0 \quad (3-1)$$

where α_i , the stoichiometric coefficient of A_i , is chosen to be positive for a product and negative for a reactant.

If C_i is the concentration of A_i at any time t , and C_{i0} its concentration at time $t = 0$, then the extent of reaction c is defined

as [3]

$$c \equiv (C_{i0} - C_i)/\alpha_i \quad (3-2)$$

During the reaction, two governing equations, namely the mass and energy balances, can be used to describe the state of the batch reactor. These well-known equations can be written as [3,11]

$$\frac{dc}{dt} = r(c,T) \quad (3-3)$$

$$C_p \frac{dT}{dt} = (-\Delta H)r(c,T) - q' \quad (3-4)$$

where $r(c,T)$, the reaction rate, is a function of c and temperature T , C_p is the total heat capacity per unit volume (including inerts), (ΔH) is the heat of reaction (negative for an exothermic reaction), and q' is the rate of heat removal.

If it is assumed that C_p is constant, then Equation (3-4) can be written as:

$$\frac{dT}{dt} = J r(c,T) - q \quad (3-5)$$

where $J \equiv (-\Delta H)/C_p$ and $q \equiv q'/C_p$

A common form of the reaction rate expression [3] is

$$r(c,T) = k_1' \exp(-E_1/RT) \prod_{i=1}^s c_i^{\beta_i} - k_2' \exp(-E_2/RT) \prod_{i=1}^s c_i^{\gamma_i} \quad (3-6)$$

where k_i' is the frequency factor, E_i is the activation energy, R is the gas constant and β_i and γ_i are the forward and backward reaction orders.

Since in the optimal control policy, the instantaneous reaction rate is a maximum, the optimal temperature schedule will be the solution of

$$\frac{\partial r(c, T)}{\partial T} = 0 \quad (3-7)$$

Thus differentiating Equation (3-6) with respect to T , gives the following optimal temperature sequence as a function of c [3]

$$T_m(c) = \frac{E_2 - E_1}{R \left[\ln \left(\frac{k_2' E_2}{k_1' E_1} \right) \prod_{i=1}^s c_i^{\xi_i} \right]} \quad (3-8)$$

where $\xi_i \equiv \gamma_i - \beta_i$ and $T_m(c)$ denotes the optimal temperature sequence.

Substituting Equation (3-8) into Equation (3-6), the corresponding maximum reaction rate is

$$r_m[c, T_m(c)] = \frac{\{[k_1' / (\rho + 1)] \prod_{i=1}^s c_i^{\beta_i \rho + 1}\}}{[(k_2' / \rho) \prod_{i=1}^s c_i^{\gamma_i \rho}]} \quad (3-9)$$

where

$$\rho \equiv E_1 / (E_2 - E_1) \quad (3-10)$$

Then from Equation (3-4) the rate of heat removal at extent c to keep the reactor on the optimal path is

$$q_m'(c) = C_p q_m(c) = \{(-\Delta H) r[c, T_m(c)]\} - C_p \frac{dT}{dt} \quad (3-11)$$

But on the optimal path

$$\frac{dT}{dt} = \frac{dT_m(c)}{dc} \frac{dc}{dt} = T'_m(c) r_m[c, T_m(c)] \quad (3-12)$$

so that

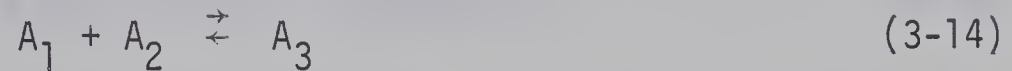
$$q'_m(c) = C_p [J - T'_m(c)] r_m[c, T_m(c)] \quad (3-13)$$

Equations (3-8), (3-9), and (3-13) will provide a straightforward computation for the optimal temperature schedule and the optimal cooling rate as a function of c .

3.2 Chien and Aris Example

3.2.1 Optimal Control Policy

Consider the hypothetical second order reversible reaction studied by Chien and Aris [5,6] with reaction mechanism



and reaction rate given by

$$r(c, T) = k_1' \exp(-E_1/RT) (3-c)(2-c) - k_2' \exp(-E_2/RT) (1+c)^2 \quad (3-15)$$

The kinetic parameters used by Chien and Aris [5,6] are:

$$\begin{array}{ll} k_1' = \exp(12) & , \quad k_2' = \exp(30) \\ E_1 = 24000 & , \quad (-\Delta H) = E_2 - E_1 = 24000 \\ J = (-\Delta H)/C_p = 400 & , \quad \rho = 1 \end{array}$$

From Equations (3-8), (3-9) and (3-13), the optimal temperature schedule is,

$$T_m(c) = \frac{E_2 - E_1}{R} \frac{1}{\left[\ln \left(\frac{k_2' E_2}{k_1' E_1} \right) \frac{(1+c)^2}{(3-c)(2-c)} \right]} \quad (3-16)$$

the maximum reaction rate is given by,

$$r_m[c, T_m(c)] = \frac{[(k_1'/2)(3-c)(2-c)]^2}{k_2'(1+c)^2} \quad (3-17)$$

and the optimal cooling rate,

$$q_m'(c) = C_p [400 - T_m'(c)] r_m[c, T_m(c)] \quad (3-18)$$

where

$$T_m'(c) = -T_m^2(c) \frac{R}{E_2 - E_1} \left[\frac{2}{1+c} - \frac{2c-5}{(3-c)(2-c)} \right] \quad (3-19)$$

Although the optimal temperature and cooling rate computations are quite straightforward, it should be noted that for small values of c the optimal temperature will be very high and may exceed the limits of safety or may require an excessively large cooling rate. When the initial state of the reactor is known and only cooling (but not heating) capacity is available, it has been shown [4,9] that the optimal control policy is a combination of an optimal cooling path and either an adiabatic path or a path with maximum cooling, depending upon the initial state of the reactor [9]. The optimal control policy is shown in Figure 3-1 where the reactor is initially operated adiabatically and then switched to the optimal cooling path after a

certain temperature is attained [5,43]. This can be explained as follows.

For adiabatic operation, $q' = 0$ and Equation (3-5) becomes

$$\frac{dT}{dt} = J r(c, T) \quad (3-20)$$

From Equations (3-3) and (3-20) it follows that

$$c = c_0 + (T - T_0)/J \quad (3-21)$$

where T_0 is the initial temperature when the extent is c_0 .

If along the adiabatic path, T is measured and the expression in Equation (3-22) is evaluated,

$$T_m [c_0 + (T - T_0)/J] - T \quad (3-22)$$

then the switch to the optimal cooling path should be made as soon as Equation (3-22) becomes zero (i.e. as soon as the reaction path intersects the switching curve).

In Equation (3-18), the optimal cooling rate is a function of c . However, in many reactions the extent cannot be directly measured while the reaction is taking place. Since temperature measurement is easier, cooling rate based on temperature (rather than extent) will be more convenient. It is known [6] that along the switching curve, the optimal temperature is monotone decreasing; consequently, Equation (3-16) can be inverted and c obtained as a function of T . Substitution of the resulting expression for c into Equation (3-18) gives the optimal cooling rate q'_m as a function of temperature.

An interesting feature which characterizes the optimal control path is the inherent self-stability when temperature measurement is used [6]. Suppose the reaction state is off the optimal path at point B in Figure 3-2 where the extent is greater than that at the optimal point, A. If the optimal rate of cooling based on the measured temperature is applied, then the state tends to change toward the optimal path. This occurs since the reaction rate at B is less than that at the corresponding optimal point, A, so that the rate of cooling is greater than the rate of heat generation. On the other hand, if the reaction state is at point C where the extent is less than the corresponding optimal point A and the optimal cooling rate based on point A is applied, then the heat generation will preponderate and again will drive the reactor state to the optimal path. By contrast if measurements of c are used to calculate the optimal cooling rate, the effect will be to drive the trajectory away from the optimal path [6].

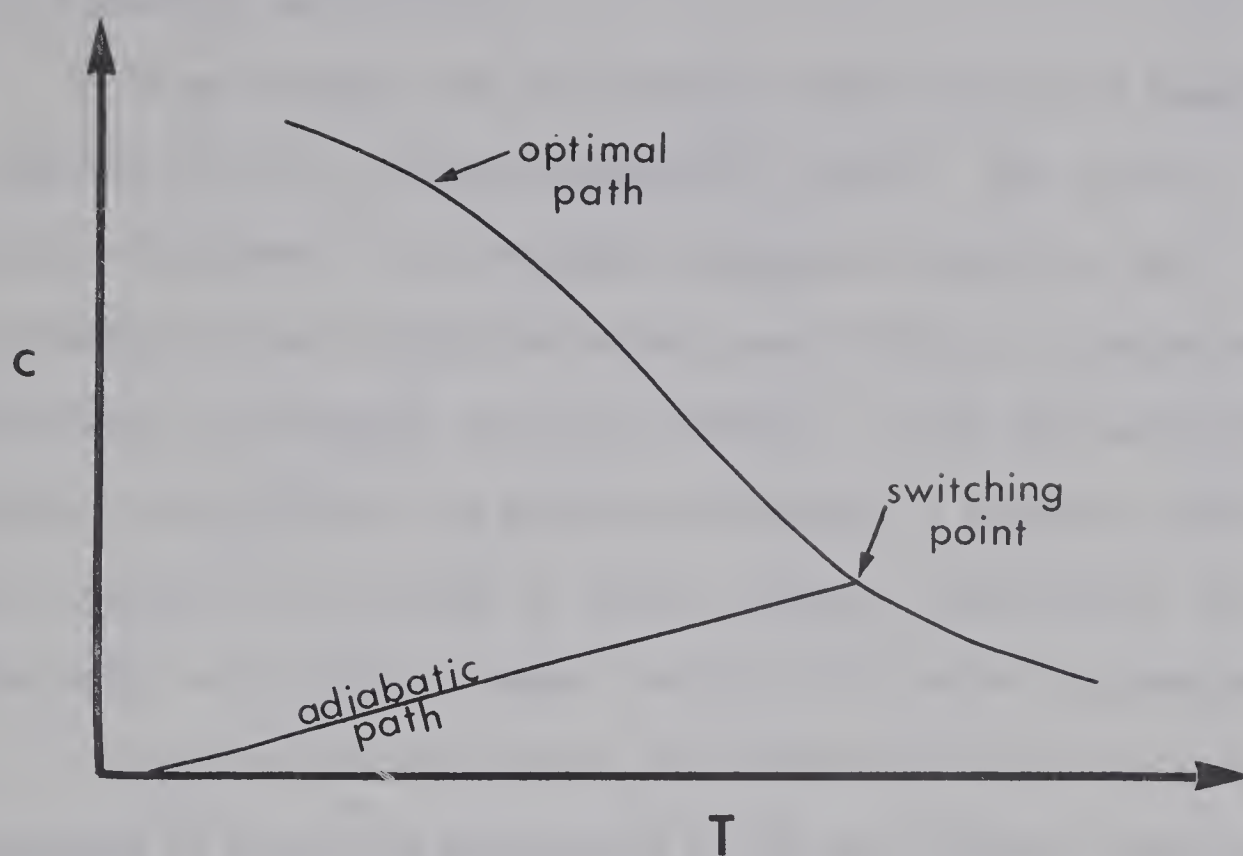


Figure 3-1 Optimal Operation for a Single Reaction Taking Place in a Batch Reactor [6]

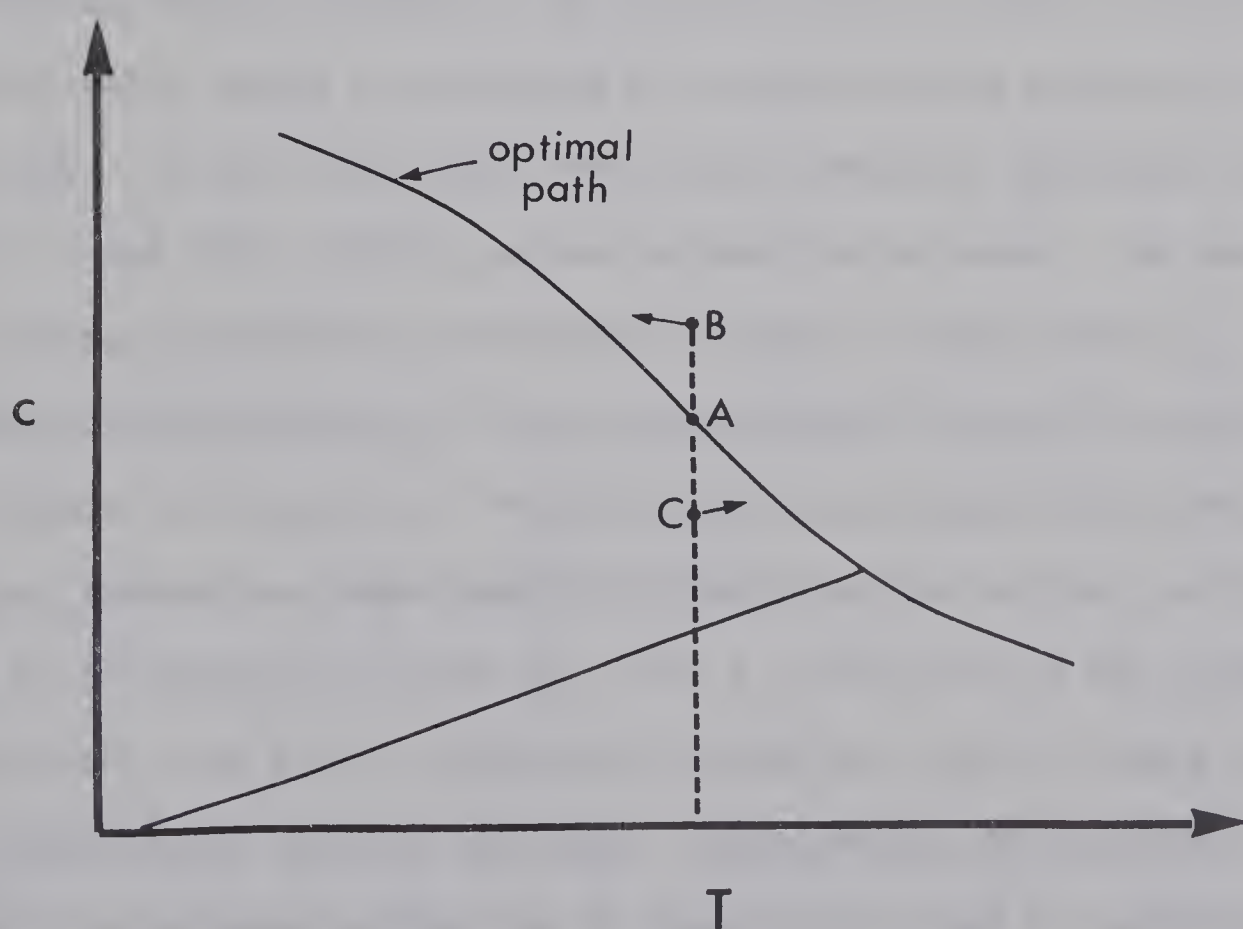


Figure 3-2 Stability of the Optimal Path [6]

3.2.2 Parameter Sensitivity

It is well-known that the optimal control policy is based on the availability of a precise mathematical model. But in real physical situations, the formulated mathematical model is only approximate and the process parameters are difficult to determine, particularly for chemical reaction systems. To see how inaccurate parameter values affect the system performance, a parameter sensitivity analysis will be made to assign accuracy requirements for a system model and to give a deeper insight into control system design.

In the previous discussion, the optimal control policy was implemented by measuring temperature along the adiabatic path and switching to the optimal cooling rate after Equation (3-22) became zero or attained a preset small value. To determine the effect of activation energy accuracy on the control policy, errors of $\pm 10\%$ in activation energy E_1 were used in calculating the optimal cooling rate. In this simulation, the initial reaction conditions are $c(0) = 0$ and $\hat{T}(0) = 500^\circ\text{K}$, and are assumed to be known. The resulting reactor trajectories are shown in Figure 3-3 when either temperature measurements or extent measurements are used to calculate the optimal cooling rate. The effect of using inaccurate values of E_1 (and temperature measurements) to calculate the optimal cooling rate is illustrated in Table 3-1. For a $+10\%$ error in the assumed value of E_1 , the time to completion is 8050 sec. which is much greater than the optimal value of 3880 sec. Consequently, the potential value of on-line parameter estimation in reducing the time to completion is readily apparent.

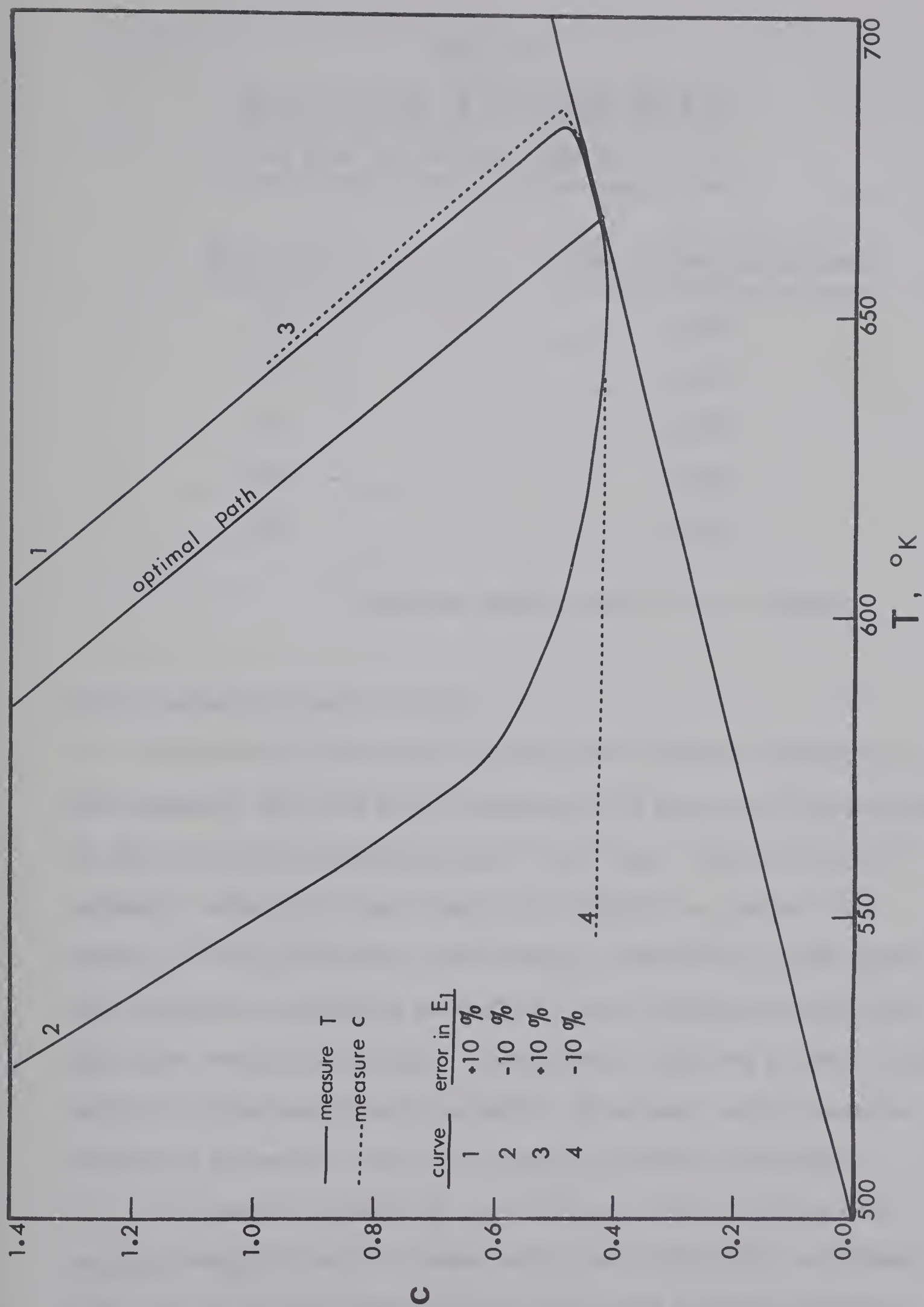


Figure 3-3 Error in Optimal Path Introduced by Calculating the Cooling Rate with $\pm 10\%$ Error in E_1

TABLE 3-1
EFFECT OF ERROR IN THE ASSUMED VALUE OF
 E_1 ON TIME TO COMPLETION (WHERE $c = 1.4$)

<u>Error in E_1 *</u>	<u>Time to Completion (sec)</u>
0	3,880
+ 1%	3,913
- 1%	3,923
+10%	8,050
-10%	16,360

* Based on nominal value of $E_1 = 24,000$

3.2.3 Suboptimal Control Policy

One of the limitations of most optimal control formulations is the assumption that the system parameters are known and time invariant. In many practical situations, this is not true. Even when nominal parameter values are known, they may be subject to change. For example, in batch reactions, the catalyst activity may change during the reaction or undetected changes in initial charge characteristics may occur from batch to batch. Consequently, when the optimal control policy is quite sensitive to parameter variations, control based on inaccurate parameter values will give poor process performance.

In chemical engineering applications, several authors have proposed feedback control schemes which are "suboptimal" and attempt to meet two main objectives [13,14,15,16]. One of the objectives is

to avoid the complicated computations required to calculate the optimal control policy, the other is to compensate for parameter changes and process environmental variations.

Here the conventional proportional control scheme proposed by Millman and Katz [13] will be investigated for the Chien and Aris reaction example. With temperature as the manipulated variable, the proportional control policy [13] is given by

$$T = K_1 + K_2 c \quad (3-23)$$

where K_1 and K_2 are constants.

By using a gradient method and repeated integration of the mass balances, Millman [12,13] determined the best values of K_1 and K_2 by assuming the kinetic parameters were known exactly and did not vary with time. His results indicate that for several batch reaction examples, the proportional control scheme resulted in a time to completion which was very close to the optimal value. However, the sensitivity of the proportional control scheme to variations in the assumed kinetic parameters was not investigated.

In the Chien and Aris example, the nonadiabatic temperature schedule, $T_m(c)$, is almost a straight line (see Figure 3-3). Thus, approximate values of K_1 and K_2 can be determined graphically to give the following suboptimal control law

$$T = 702 - 84 c \quad (3-24)$$

Simulation results showed that if Millman's control scheme in Equation (3-24) was initiated at the adiabatic switching point, a

completion time of 3885 sec. would result. This value is very close to the optimal value of 3880 sec. as indicated in Table 3-1. If the extent of reaction is measurable or can be estimated, this control policy seems to be quite effective.

Optimal cooling rate based on an incorrect value of the activation energy E_1 can result in poor reactor control as has been shown in Section 3.2.2. Hence, cooling rate based on an optimal policy is not feasible when changes in activation energy E_1 occur and are not detected. To determine how the proportional control policy works when the actual (rather than the assumed) value of E_1 changes, simulated results of optimal and proportional control strategies are shown in Table 3-2. It is remarkable that the proportional control policy in Equation (3-24) results in completion times which are within 1% of the optimal values despite the occurrence of 10% changes in E_1 . By contrast, the sensitivity of the optimal control policy to parameter variation is again apparent from Table 3-2. In these optimal control calculations (and the ones to follow), the cooling rate is calculated from temperature measurements.

TABLE 3-2
EFFECT OF VARIATIONS IN THE ACTUAL VALUE OF
 E_1 ON CONTROL SCHEMES

<u>Control</u>	<u>Variation in E_1^*</u>	<u>Time to Completion(sec)</u>
optimal based on actual value of E_1	-10%	473
"	+10%	32,685
optimal based on nominal value of E_1	-10%	1,046
"	+10%	132,123
proportional based on nominal value of E_1	-10%	473
"	+10%	32,830

* Based on the nominal value of $E_1 = 24,000$

Thus it appears that the proportional control policy can compensate for variation of parameters even when the changes are not detected. However, if the extent c cannot be readily measured, some type of on-line state estimation would be required. This topic is considered in the next section.

3.3 Sequential State and Parameter Estimation

3.3.1 Parameter Estimation

Optimal and proportional control policies have been investigated for the Chien and Aris reaction example. Parameter sensitivity calculations showed that an incorrect value of E_1 will result in poor

reactor control if the optimal cooling policy is used. In Millman's method [12,13], the calculation of constants K_1 and K_2 in Equation (3-23) is based on assumed process parameter values, and is quite insensitive to changes in E_1 . However, Millman's method requires that an estimate (or measurement) of the extent of reaction must be available.

With reactor operation divided into an adiabatic path and a optimal path as shown in Figure 3-1, Chien and Aris [5] used numerical approximation of the time derivative of temperature (i.e. dT/dt in Equation (3-20)) and matrix inversion least squares technique to identify the unknown parameters during the adiabatic path.

Ray and Aris [7] used the same technique to identify unknown parameters from several isothermal runs then switched to a non-isothermal path (i.e. optimal path in Figure 3-1). This latter approach will result in some degree of suboptimality in the whole process. One common problem to both approaches is the large round-off computation errors encountered as the determinant of the matrix to be inverted becomes very small. Their methods have the advantage that initial guesses of the parameters are not required. However, their methods also suffered two main shortcomings. One is that the computation scheme cannot easily be extended to a complex reaction scheme, since in this case nonlinear regression techniques would normally be required. The other disadvantage is that the accuracy of the required data is quite high so when the measurement noise is high (even for a measurement error of 1°C), their methods will not provide satisfactory estimates.

As an alternative approach, the Detchmندی and Sridhar nonlinear filter technique [22] can be used to perform parameter estimation during the adiabatic path. Suppose E_1 is the only undetermined parameter in this example and assume no dynamic errors are involved in the process. It will also be assumed that temperature, but not extent, can be measured and that the noisy temperature data, $y(t)$, can be represented as

$$y(t) = T(t) + \varepsilon(0, \sigma) \quad (3-25)$$

where the measurement errors $\varepsilon(0, \sigma)$ are assumed to be Gaussian distributed with zero mean and an appropriate standard deviation, σ .

One of the difficulties involved in parameter estimation by a nonlinear filter technique is that the filter differential equations are often stiff, i.e. the eigenvalues differ greatly in magnitude [45, 14]. To reduce this difficulty, Seinfeld and Chen [14] proposed defining new variables, containing the unknown parameters, which are of the same order of magnitude as the states. To reduce the stiffness effect in this example, the state variables of the filter are defined as

$$\hat{x}_1(t) = \hat{c}(t) \quad (3-26)$$

$$\hat{x}_2(t) = \frac{\hat{T}(t) - 500}{100} \quad (3-27)$$

$$\hat{x}_3(t) = \frac{\hat{E}_1(t) - E_{1,ref}}{E_{1,ref}} \quad (3-28)$$

where $\hat{c}(t)$ is the estimated extent, $\hat{E}_1(t)$ and $\hat{T}(t)$ are the estimated

activation energy and temperature, and $E_{1,ref}$ is a specified reference value.

Then the filter equations (2-8 to 2-10) can be developed with the following state functions and Jacobian applicable during the adiabatic path:

$$f_1 = k_1' \exp[-(\hat{E}_1(t)/R)/\hat{T}(t)](3-\hat{x}_1)(2-\hat{x}_1) - k_2' \exp[-(\frac{\hat{E}_1(t)+24000}{R})/\hat{T}(t)](1+\hat{x}_1)^2 \quad (3-29)$$

$$f_2 = 400 f_1 \quad (3-30)$$

$$f_3 = 0 \quad (3-31)$$

$$f_{11} = k_1' \exp[-(\hat{E}_1(t)/R)/\hat{T}(t)](-5 + 2\hat{x}_1) - 2k_2' \exp[-(\frac{\hat{E}_1(t)+24000}{R})/\hat{T}(t)](1+\hat{x}_1) \quad (3-32)$$

$$f_{12} = \{k_1' \exp[-(\hat{E}_1(t)/R)/\hat{T}(t)](\frac{\hat{E}_1(t)}{R})(3-\hat{x}_1)(2-\hat{x}_1) - k_2' \exp[-(\frac{\hat{E}_1(t)+24000}{R})/\hat{T}(t)](\frac{\hat{E}_1(t)+24000}{R})(1+\hat{x}_1)^2\}(\frac{100}{\hat{T}(t)^2}) \quad (3-33)$$

$$f_{13} = \{k_1' \exp[-(\hat{E}_1(t)/R)/\hat{T}(t)](3-\hat{x}_1)(2-\hat{x}_1) - k_2' \exp[-(\frac{\hat{E}_1(t)+24000}{R})/\hat{T}(t)](1+\hat{x}_1)^2\}(-\frac{E_{1,ref}}{R\hat{T}(t)}) \quad (3-34)$$

$$f_{21} = 400 f_{11} \quad (3-35)$$

$$f_{22} = 400 f_{12} \quad (3-36)$$

$$f_{23} = 400 f_{13} \quad (3-37)$$

$$f_{31} = f_{32} = f_{33} = 0 \quad (3-38)$$

with

$$\hat{E}_1(t) = E_{1,\text{ref}} + \hat{x}_3(t) E_{1,\text{ref}} \quad (3-39)$$

$$\hat{T}(t) = 500 + 100 \hat{x}_2(t) \quad (3-40)$$

Suppose the initial reactor state, $c = 0$ and $T = 500$ at $t = 0$, is known exactly and $E_{1,\text{ref}}$ is chosen to be 24000 (the actual value of E_1); then if the initial estimate of E_1 is 10% low (i.e. $\hat{E}_1(0) = 21600$), the initial states of the filter are

$$\hat{x}_1(0) = 0, \quad \hat{x}_2(0) = 0, \quad \hat{x}_3(0) = -0.1$$

As discussed in Section 2.2, numerical experimentation is required to determine a satisfactory initial covariance matrix $\underline{\underline{P}}(0)$. For the first trial run, the matrix $\underline{\underline{P}}(0)$ was arbitrarily set equal to the identity matrix. Additional trials indicated that a diagonal $\underline{\underline{P}}(0)$ matrix was adequate providing that the element corresponding to the unknown parameter is chosen to be larger than the corresponding diagonal elements for the states. After 10 trials, the following initial covariance matrix $\underline{\underline{P}}(0)$ was finally selected

$$\underline{\underline{P}}(0) = \begin{bmatrix} 0.0025 & 0 & 0 \\ 0 & 0.01 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Thus with $\underline{\underline{P}}(0)$ specified and the initial state available, simulation of the process estimation was performed by integrating the filter equations with a Runge-Kutta-Gill 4th order routine [43] using a data sampling interval of $t_s = 1$. The process data were generated by integrating Equations (3-5) and (3-25) with the same integration routine and an integration step size of 0.5 sec. The noise data was generated by a standard Gaussian random number generator with a standard deviation of $\sigma = 0.1$ and zero mean.

Figure 3-4 shows the estimate of E_1 obtained using the standard full filter (Filter I) when the assumed values of $\hat{E}_1(0)$ contain 10% errors. The parameter estimation is judged to be quite satisfactory since convergence was obtained before the switching time of 1695 sec.; i.e. after $t > 1695$ sec. the adiabatic operation is replaced by optimal cooling which requires an estimate of E_1 .

In order to evaluate the performance of the piecewise recursive filter algorithm (Filter II) as discussed in Section 2.3, the update interval for the covariance differential equation was chosen to be $t_p = 10$ (i.e. 10 times the data sampling interval). Then with the same initial state and initial covariance matrix $\underline{\underline{P}}(0)$ as used in Filter I, the process is simulated under the same conditions of Figure 3-4. Results are shown in Figure 3-5. In comparison with Figure 3-4 for the Filter I estimation, the Filter II estimation

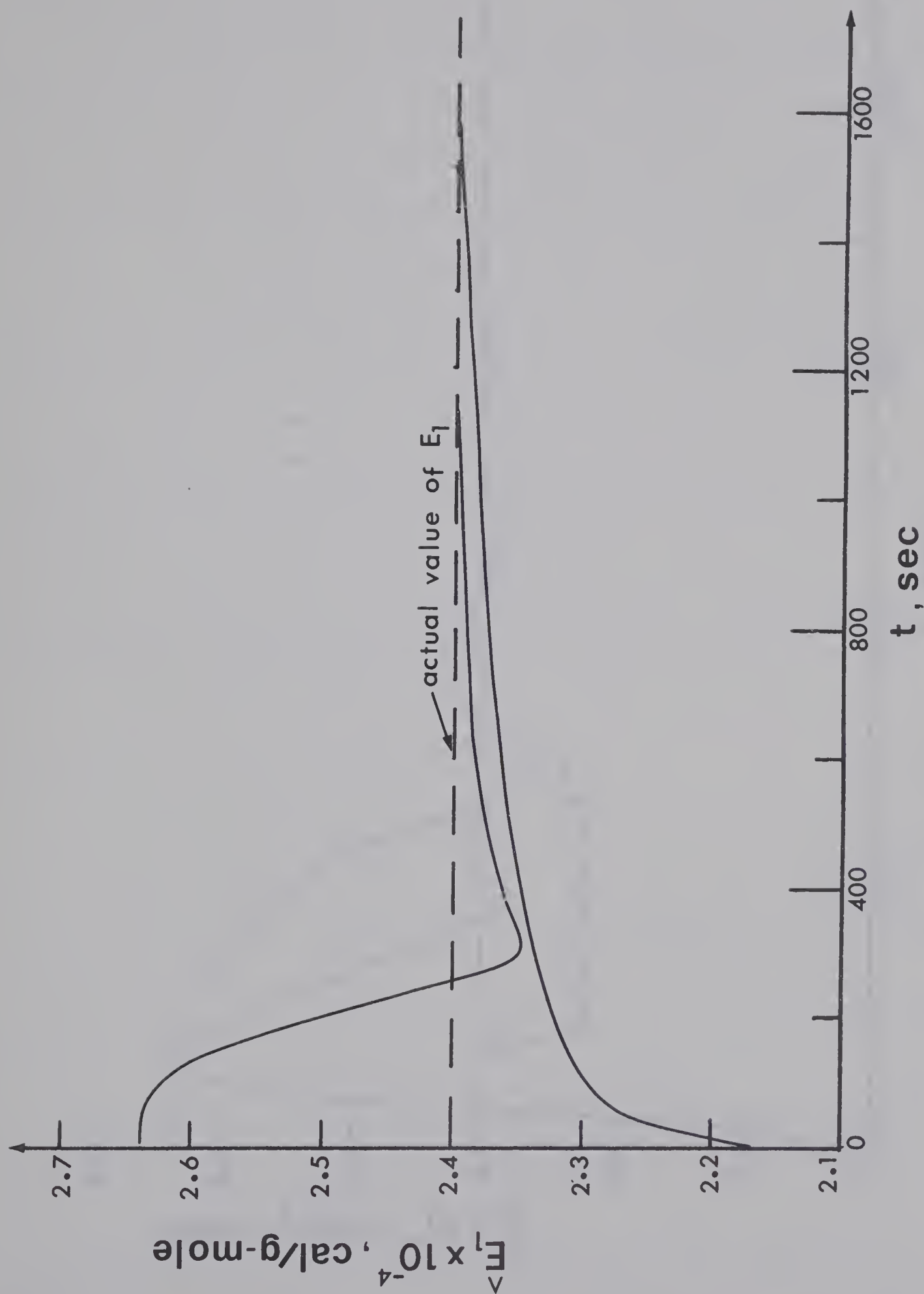


Figure 3-4 Filter I Estimation of E_1 with $\pm 10\%$ Error in $\hat{E}_1(0)(t_s = 1 \text{ sec.}, \sigma = 1^\circ\text{C})$

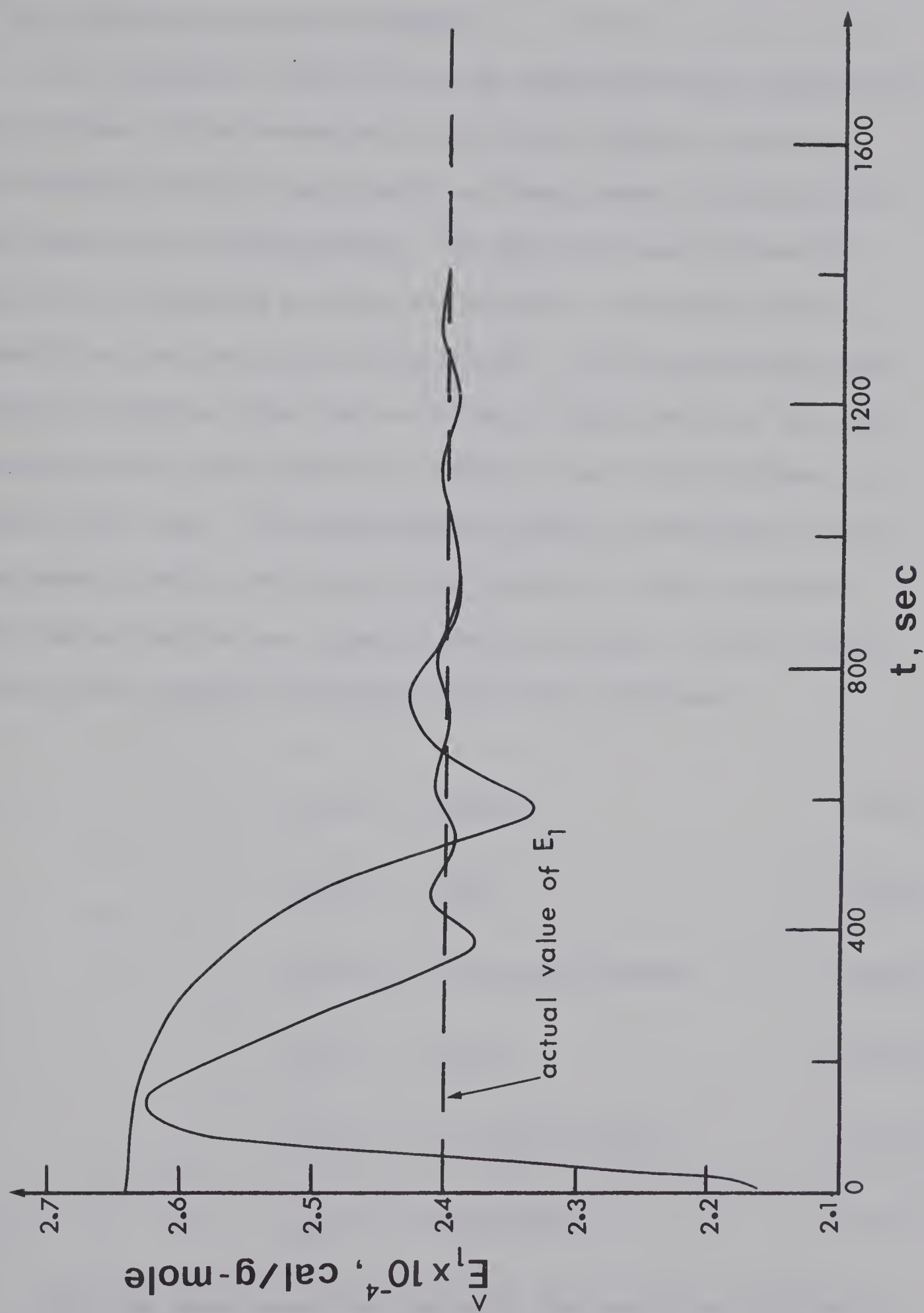


Figure 3-5 Filter II Estimation of E_1 with $\pm 10\%$ Error in $\hat{E}_1(0)(t_s = 1 \text{ sec.}, \sigma = 1^\circ\text{C}, t_p = 10 t_s)$

shows a more rapid convergence. Hence the Filter II algorithm appears to be a promising estimation scheme.

As discussed in Section 2.4, the computation time required for the nonlinear filter technique is a critical factor in real-time applications because integration of a large number of differential equations is very time-consuming. If the covariance differential equations are replaced by algebraic equations, then the saving in computation time can be quite significant. In choosing appropriate algebraic equations, the time variation of each element of the covariance matrix using Filter I or Filter II was first obtained for several trial runs. Then approximate algebraic expressions of the same general shape were assumed, and improved by trial and error until the estimation was judged to be satisfactory. In this manner, the following algebraic equations were finally obtained.

$$P_{11}(t) = 0.0025 \quad (3-41)$$

$$P_{12}(t) = 0.007 \quad (3-42)$$

$$P_{13}(t) = -0.04 \exp(-0.0016t) \quad (3-43)$$

$$P_{22}(t) = 0.0023 \quad (3-44)$$

$$P_{23}(t) = -0.1 \exp(-0.0016t) \quad (3-45)$$

$$P_{33}(t) = \exp(0.003t) \quad (4-51)$$

With the above equations replacing the covariance differential equations in Filter I, the process was simulated with the previously

used initial state and noise level. For ease of reference, the above filter with algebraic expressions for the elements of $\underline{P}(t)$ will be referred to as Filter III. Figure 3-6 shows the estimation of E_1 by Filter III. It is found that the Filter III estimation of E_1 is better than the estimates provided by Filter I and Filter II. Figure 3-7 compares the estimation of c obtained using the three filter algorithms when $\hat{E}_1(0)$ contains a -10% error. A comparison of Figure 3-4 and 3-7 indicates that a good estimate of c occurred when a good estimate of E_1 was obtained, as would be expected. Table 3-3 compares the effect of $\hat{E}_1(0)$ on the final estimates of E , c and T . Even with 20% errors in $\hat{E}_1(0)$, the estimation of E_1 by the simplified algorithms, Filters II and III are still quite encouraging. The poor estimation of extent c by the Filter II algorithm when $\hat{E}_1(0)$ contains a +20% error is due to slower convergent rate of the estimated E_1 , since when E_1 is higher the reaction is proceeding slower, and hence the estimated $\hat{c}$ is lower than the actual extent.

From the above results, the simplified nonlinear filter estimation, seems to be a feasible approach, particularly since the full filter, Filter I, is "suboptimal" to begin with due to approximations made during its derivation.

3.3.2 Effect of Update Interval, t_p , on Filter II Estimation

In the above simulation, the update interval for the covariance differential equation, $t_p = 10$, was chosen quite arbitrarily. In actual applications, large values of t_p are desirable to reduce computational requirements. However, if t_p is too large the estimation

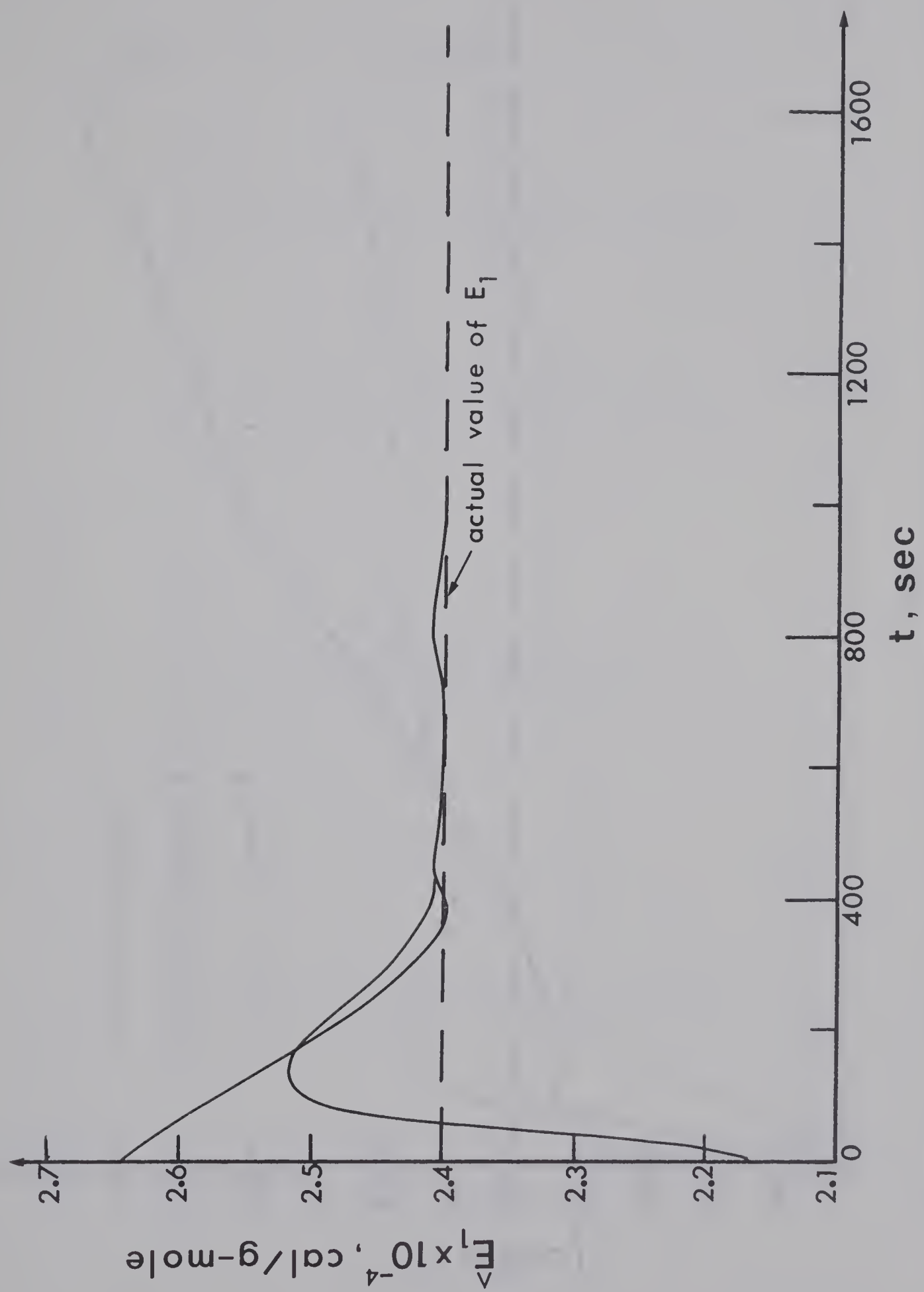


Figure 3-6 Filter III Estimation of E_1 with $\pm 10\%$ Error in $\hat{E}_1(0)$ ($t_s = 1 \text{ sec.}, \sigma = 1^\circ\text{C}$)

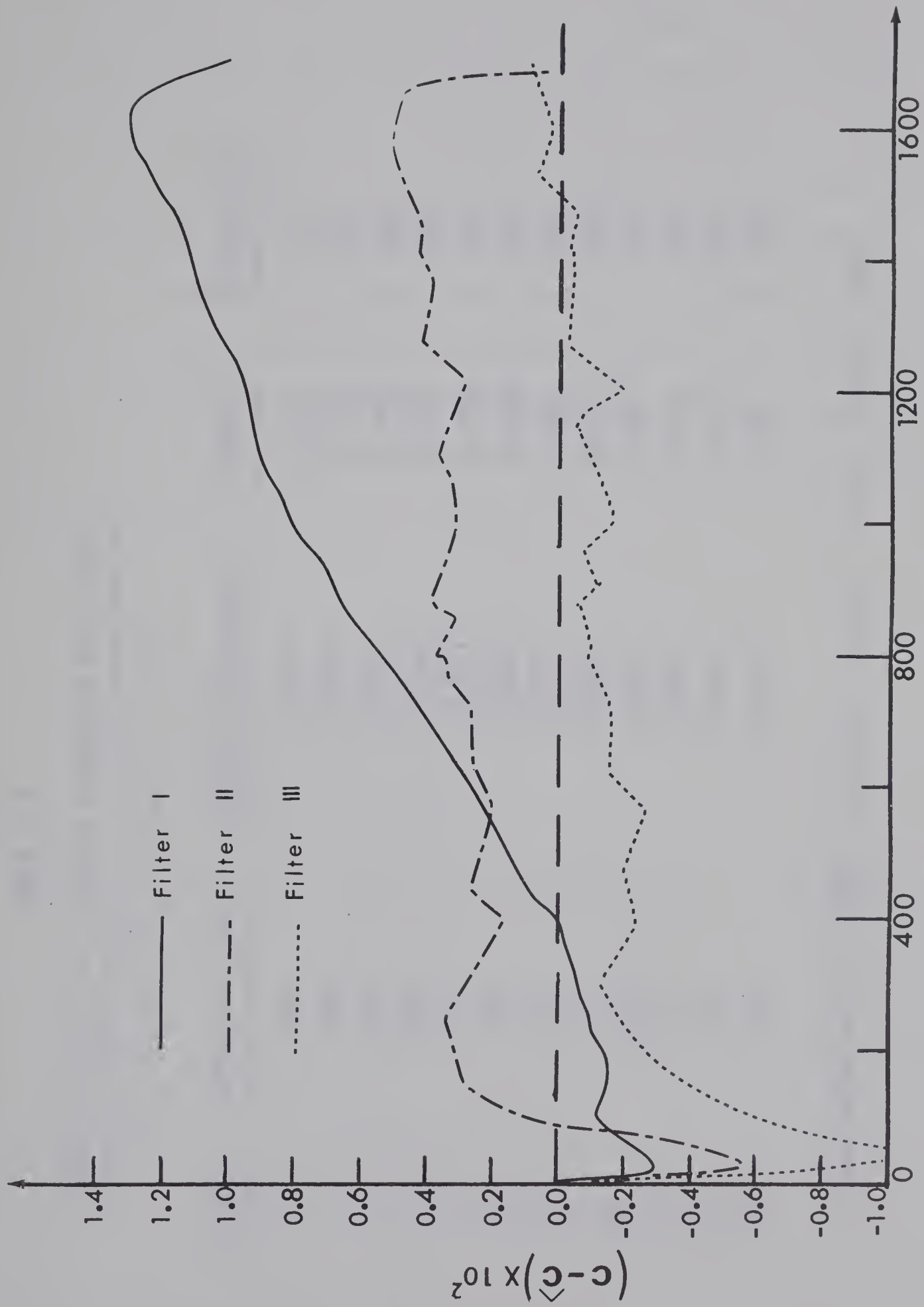


Figure 3-7 Estimation of Extent c by Three Filters with -10% Error in $\hat{E}_1(0)(t_s = 1 \text{ sec.}, \sigma = 1^\circ\text{C})$

TABLE 3-3

EFFECT OF $\hat{E}_1(0)$ ON ESTIMATED PARAMETER AND STATES $(t_s = 1 \text{ sec.}, t_p = 10 \text{ sec.}, \sigma = 1^\circ\text{C})$

Filter	Error in $\hat{E}_1(0)$	$\hat{E}_1(1695)(\text{cal/g-mole})$	$\hat{c}(1695)^*$	$\hat{T}(1695)(^\circ\text{K})^*$
I	+10%	24,007	0.414	667
I	-10%	23,970	0.410	670
I	+20%	23,355	0.448	686
I	-20%	22,749	0.415	694
II	+10%	24,043	0.404	667
II	-10%	24,006	0.420	667
II	+20%	24,112	0.365	667
II	-20%	23,999	0.421	668
III	+10%	23,992	0.421	667
III	-10%	23,997	0.418	668
III	+20%	23,987	0.423	667
III	-20%	23,983	0.426	667

* True value for $E_1 = 24000 \text{ cal/g-mole}$: $c(1695) = 0.419$, $T(1695) = 666^\circ\text{K}$

may not converge. Table 3-4 compares the effect of t_p on the Filter II estimates at the switching time of $t = 1695$ sec. Even with $t_p = 100$, the Filter II algorithm still provides a good parameter estimate although the estimated extent, $\hat{c}(1695)$, deviates farther from the actual value of $c(1695) = 0.419$ as t_p increases. This is due to the fact that when t_p is increased, the resulting slower convergence rate of estimated E_1 produces a poor estimate of extent c . A further check calculation with $t_p = \infty$, i.e. $\underline{\underline{P}}(t) = \underline{\underline{P}}(0)$ for all $t > 0$, showed that the estimate of E_1 did not change greatly from the assumed value of $\hat{E}_1(0)$ and the estimated extent c is lower than the actual extent, as would be expected.

TABLE 3-4
EFFECT OF t_p ON PERFORMANCE OF FILTER II

$$(\hat{E}_1(0) = 26400 \text{ cal/g-mole}, t_s = 1 \text{ sec.}, \sigma = 1^\circ\text{C})$$

<u>$\hat{E}(1695)(\text{cal/g-mole})$</u>	<u>$\hat{c}(1695)^*$</u>	<u>$\hat{T}(1695)(^\circ\text{K})^*$</u>	<u>$t_p(\text{sec})$</u>
24,043	0.404	667	10
23,909	0.384	668	50
23,988	0.367	668	100

* Actual values for $E_1 = 24000$ cal/g-mole:

$$c(1695) = 0.419, \quad T(1695) = 666^\circ\text{K}$$

3.3.3 Comparison of Computation Times

To evaluate how much computation time can be saved by using a simplified filter algorithm, object decks for the Fortran program were generated for all three filter algorithms and estimates of computation times were obtained for an IBM 360/67 computer with the MTS operating system. Table 3-5 gives an appropriate comparison, where the indicated time is the CPU time for the computer program. It is found that the CPU time can be reduced by 58% by using Filter II with $t_p = 10$, and by 60% using Filter III in comparison with the Filter I estimation. Since CPU time includes both program I/O and computation times, it is difficult to estimate what percentage of CPU time is concerned with the computation time.

TABLE 3-5

COMPARISON OF COMPUTATION TIMES FOR THE FILTER ALGORITHMS*

$$(\hat{E}_1(0) = 26400 \text{ cal/g-mole}, t_s = 1 \text{ sec.}, \sigma = 1^\circ\text{C})$$

<u>Filter</u>	<u>Computation Time (sec)</u>	<u>t_p(sec)</u>
I	49.3	-
II	20.7	10
II	18.1	50
II	18.0	100
III	19.6	-

*This value includes I/O operations.

3.3.4 Effect of Initial State Estimate

In some physical situations, the initial state is not known exactly. For example, the properties of the initial charge to a batch reactor may change in an unanticipated manner, particularly when the reactants are supplied from other units in the plant. To see how an inaccurate initial state estimate affects the filter performance, the reaction example is simulated with initial estimates of $\hat{c}(0) = 0.01$, $\hat{E}_1(0) = 26400$ and two values of $\hat{T}(0)$, 490°K and 510°K . In this simulation the previously used initial covariance matrix $\underline{P}(0)$ was used for both Filter I and II algorithms. Table 3-6 lists the estimated states at the switching time while Figure 3-8 shows the response of the estimated activation energy, $\hat{E}_1(t)$. The response is consistent with physical intuition. At the beginning of the reaction $c(0) = 0$ and $T(0) = 500^\circ\text{K}$ but the estimated values are $\hat{c}(0) = 0.01$ and $\hat{T}(0) = 510^\circ\text{K}$; consequently, the estimated E_1 increases initially to make the estimated $\hat{c}(t)$ and $\hat{T}(t)$ become closer to the actual extent and temperature. Finally, when $\hat{c}(t)$ and $\hat{T}(t)$ approach the actual values of $c(t)$ and $T(t)$, the estimated activation energy, $\hat{E}(t)$, converges to the actual value. As before, better parameter estimates are obtained by using simplified algorithms, especially Filter II in this case.

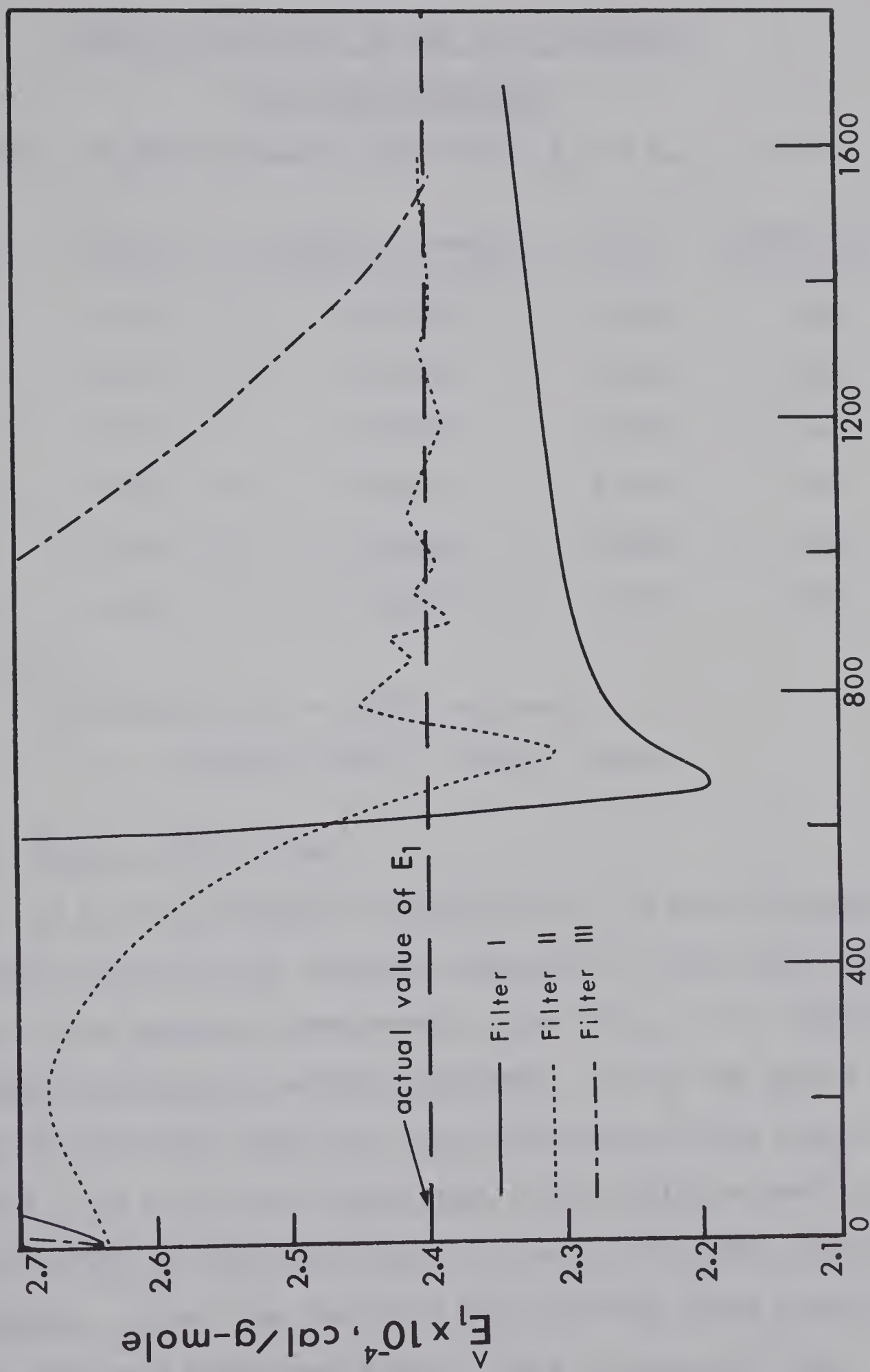


Figure 3-8 Effect of Inaccurate Initial State Estimate on Estimation of E_1 with -10% Error
in $\hat{E}_1(0)$, $\hat{c}(0) = 0.01$ and $\hat{T}(0) = 510^\circ\text{K}$ ($t_s = 1$ sec., $\sigma = 1^\circ\text{C}$)

TABLE 3-6
EFFECT OF INCORRECT INITIAL STATE ESTIMATES
ON FILTER PERFORMANCE

$(\hat{E}_1(0) = 26,400 \text{ cal/g-mole}, \hat{c}(0) = 0.01, t_s = 1 \text{ sec.}, \sigma = 1^\circ\text{C})$

<u>Filter</u>	<u>$\hat{T}(0)(^\circ\text{K})$</u>	<u>$\hat{E}_1(1695)(\text{cal/g-mole})$</u>	<u>$\hat{c}(1695)^*$</u>	<u>$\hat{T}(1695)^*(^\circ\text{K})$</u>
I	510	23,385	0.453	685
I	490	23,331	0.454	686
II	510	24,030	0.408	667
II	490	24,011	0.417	667
III	510	24,016	0.444	668
III	490	23,923	0.453	666

* True value for $E_1 = 24,000 \text{ cal/g-mole}$

$c(1695) = 0.419, T(1695) = 666^\circ\text{K}$

3.3.5 Effect of Noise Level

As has been discussed in Section 3.3.1, the method developed by Chien and Aris [5] for parameter estimation is quite sensitive to noise in the temperature measurements. Even with $\sigma = 1^\circ\text{C}$, they did not obtain satisfactory parameter estimates. To see how large a noise level the nonlinear filter can allow, the effect of noise level on Filters I, II and III was investigated. From simulation results, it was found that a large noise level will result in a slowly convergent estimation. It was also found that the simplified filter algorithms can handle large measurement errors. Table 3-7 shows the final

estimates of E , c and T by Filters I, II and III.

When $\hat{E}_1(0)$ has -10% error and $t_s = 1$, the Filter I estimation scheme "blew up" because of numerical instability in the filter equations. When the estimated activation energy, $\hat{E}_1$, is too low, the fixed integration step size of 1 sec. gave large computation errors especially in the evaluation of the Jacobian. As a further check, calculations were made by using a data sampling time of $t_s = 0.5$ sec. for the Filter I estimation when $\hat{E}_1(0)$ has a -10% error involved and $\sigma = 10^\circ\text{C}$. As indicated in Table 3-7, for $t_s = 0.5$ the numerical instability was eliminated and the estimation converged.

From a practical point of view, $\sigma = 10^\circ\text{C}$ represents a large temperature measurement error and so higher noise levels were not investigated.

3.3.6 Effect of Data Sampling Interval

In all the previous calculations, a data sampling time of $t_s = 1$ was assumed for the temperature measurements. In real-time applications, large sampling intervals are desirable to reduce the loading on the computer. However, if the sampling interval is too large, the filter may yield poor estimates. To test the "robustness" of the filter algorithms, a data sampling time of $t_s = 10$ was investigated. The standard set of conditions of $\hat{c}(0) = 0$, $\hat{T}(0) = 500$, $\sigma = 1^\circ\text{C}$ and the same $\underline{p}(0)$ were used as before. Figures 3-9 and 3-10 show the estimated responses with -10% and +10% errors involved in $\hat{E}_1(0)$, respectively. When compared with the filter estimation for $t_s = 1$ as shown in Figures 3-4, 3-5 and 3-6, the convergence rates

TABLE 3-7

EFFECT OF NOISE ON FILTER PERFORMANCE

 $(\hat{c}(0) = 0, \hat{T}(0) = 500^\circ\text{K}, t_s = 1 \text{ sec.})$

Filter	$\sigma(^{\circ}\text{C})$	Error in $\hat{E}_1(0)$	$\hat{E}(1695)(\text{cal/g-mole})$	$\hat{c}(1695)^*$	$\hat{T}(1695)^*(^{\circ}\text{K})$
I	1	+10%	24,007	0.414	667
I	1	-10%	23,970	0.410	670
I	10	+10%	23,963	0.421	672
I***	10	-10%	23,827	0.409	676
II**	1	+10%	24,043	0.404	667
II**	1	-10%	24,006	0.420	667
II**	10	+10%	24,062	0.401	667
II**	10	-10%	24,051	0.417	667
III	1	+10%	23,992	0.421	667
III	1	-10%	23,997	0.418	668
III	10	+10%	23,894	0.435	673
III	10	-10%	23,895	0.435	673

* True value for $E_1 = 24,000 \text{ cal/g-mole}$: $c(1695) = 0.419, T(1695) = 666^\circ\text{K}$ ** $t_p = 10 \text{ sec.}$ *** $t_s = 0.5 \text{ sec.}$

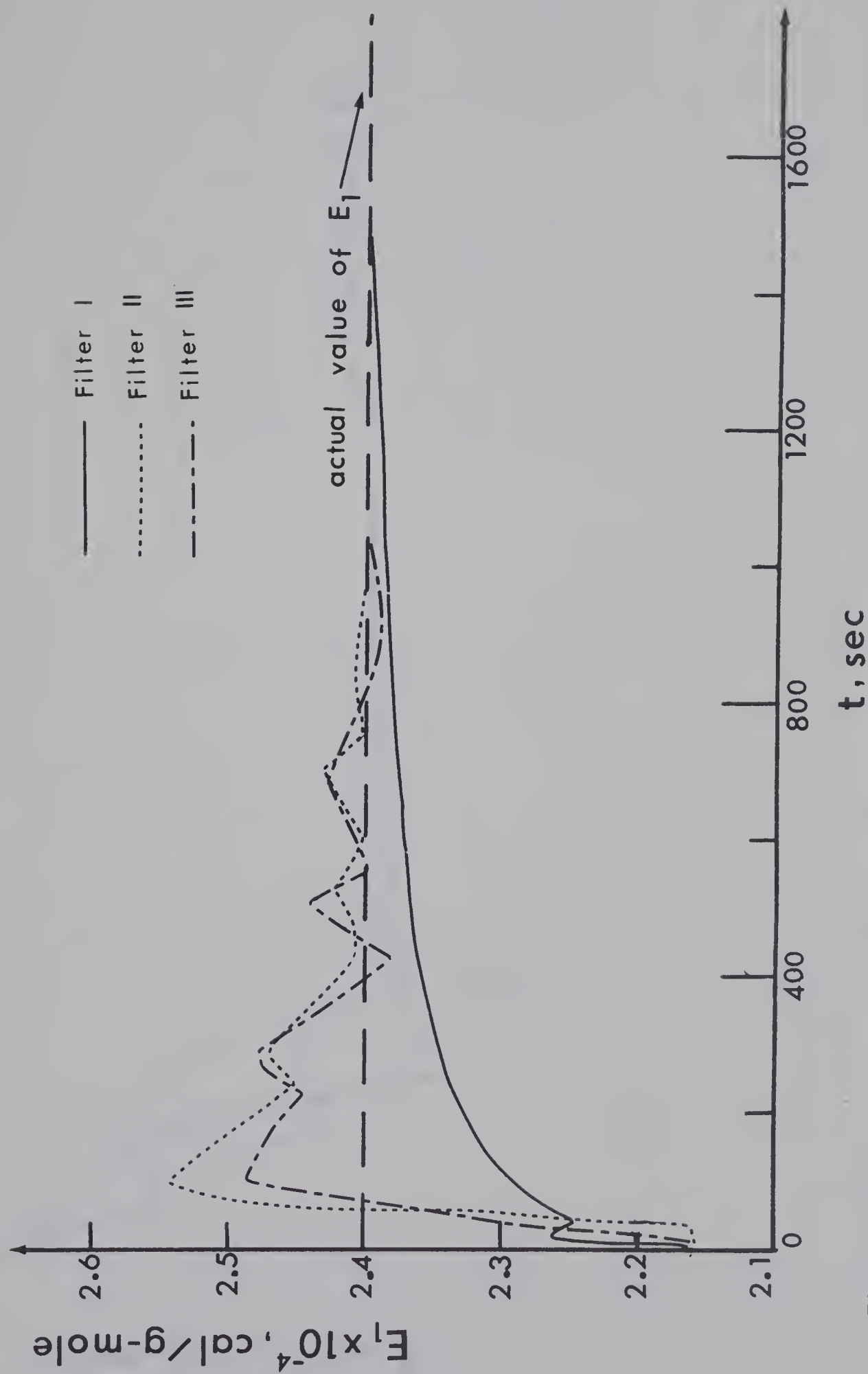


Figure 3-9 Comparison of E_1 Estimation Obtained when $t_s = 10$ sec. ($\hat{c}(0) = 0$, $\hat{T}(0) = 500^\circ\text{K}$, $\hat{E}_1(0) = 21,600$ cal/g-mole, $\sigma = 1^\circ\text{C}$)

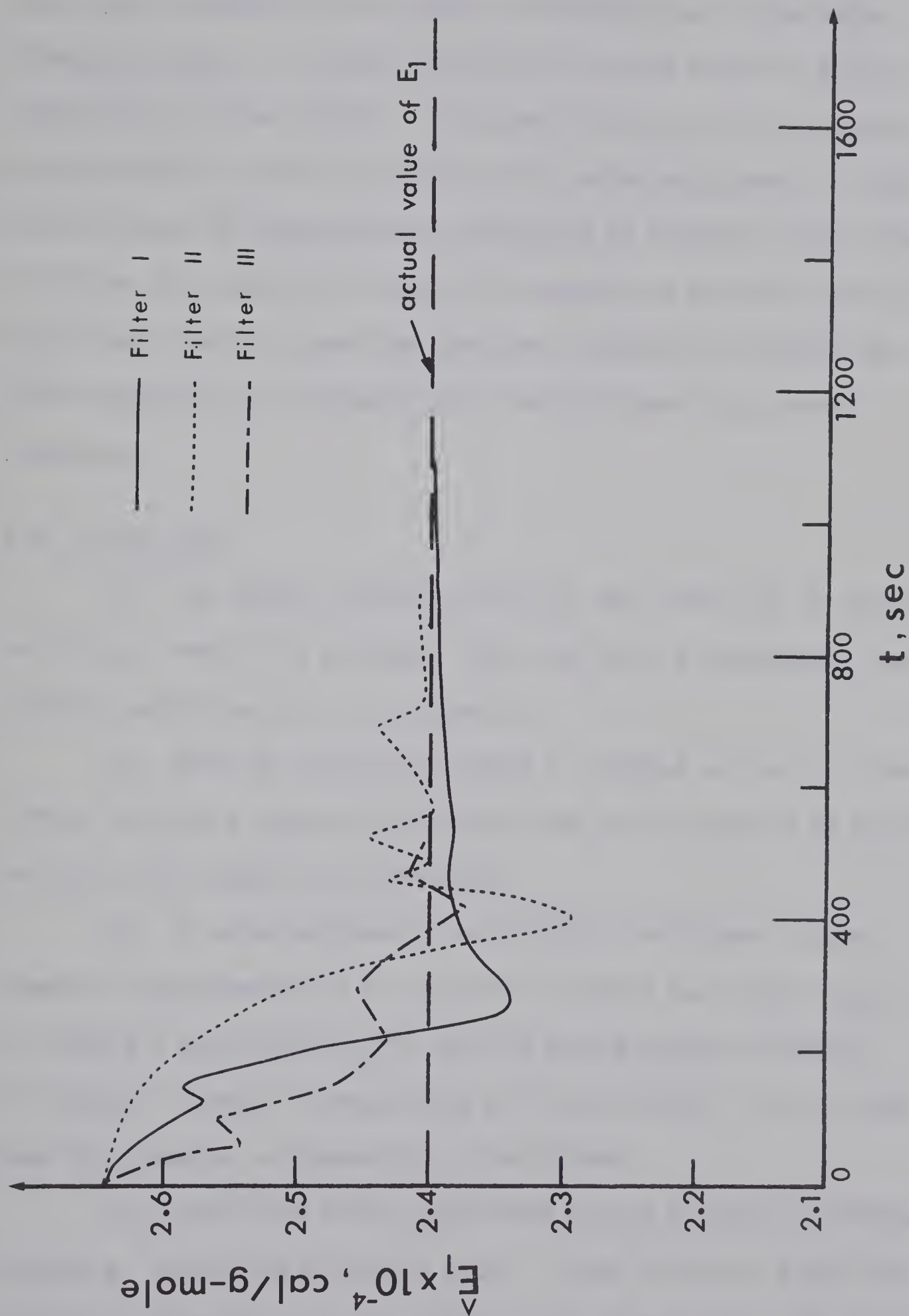


Figure 3-10 Comparison of E_1 Estimation Obtained when $t_s = 10 \text{ sec}$. ($\hat{c}(0) = 0$, $\hat{T}(0) = 500^\circ\text{K}$, $\hat{E}_1(0) = 26,400 \text{ cal/g-mole}$, $\sigma = 1^\circ\text{C}$)

of E_1 estimation are essentially the same, although large computation errors are involved in the filter calculations due to the large integration step. A further calculation with an error in $\hat{E}_1(0)$ of -10% and $t_s = 15$ was checked. Both the Filter I and II estimates become unstable, while Filter III still worked quite well. Since more differential equations are integrated in Filters I and II than in Filter III, numerical instabilities appear to be more critical in the Filter I and II algorithms when the integration step for the filter equations is increased (i.e. the data sampling interval increases).

3.4 Conclusions

(1) The optimal control policy is very sensitive to parameter variation. Hence if a parameter does vary and is undetected, the optimal control policy is not feasible.

(2) When the activation energy E_1 changed and was not identified, Millman's proportional control law still seems to be practical, providing the extent can be measured.

(3) In using Detchmندی and Sridhar's nonlinear filter, numerical experimentation is required to find a satisfactory $\underline{\underline{P}}(0)$. In finding a satisfactory $\underline{\underline{P}}(0)$ for the single reaction example, the diagonal element corresponding to the parameter is much larger than the elements corresponding to the states.

(4) Simplified filter algorithms can be applied to estimate unknown E_1 during the adiabatic path. It was found the simplified nonlinear algorithms are less sensitive to noise level, data sampling

time and error in the initial state estimate.

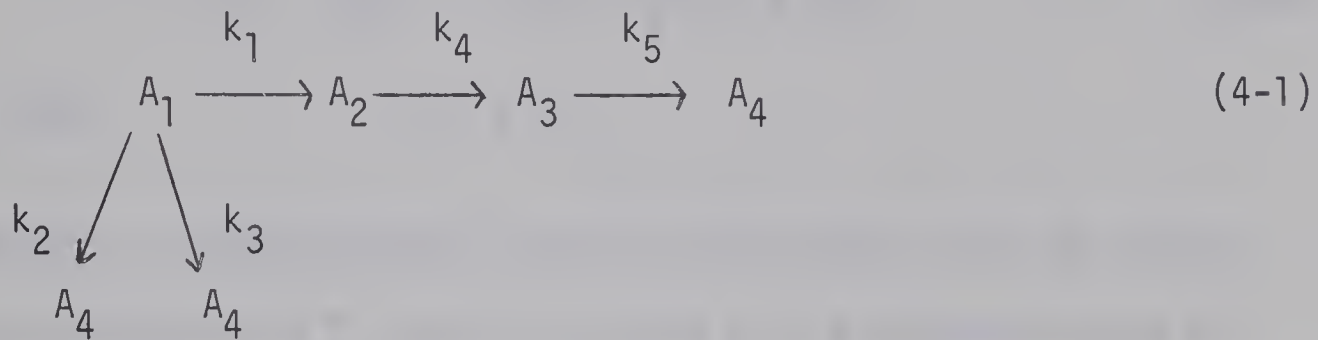
(5) To find a set of satisfactory algebraic equations for the Filter III algorithm, one approach is to find the response of all elements of $\underline{\underline{P}}(t)$ for a Filter I or II simulation, then exponential expressions can be used as approximations to these responses. Since the response of $\underline{\underline{P}}(t)$ depends on different initial estimates of states (including the initial estimate of unknown parameter), the responses of $\underline{\underline{P}}(t)$ are required for several initial state estimates in order to obtain satisfactory algebraic equations for Filter III.

CHAPTER IV

STUDIES OF A COMPLEX REACTION

4.1 Formulation

Consider the complex batch reaction originally studied by Rosenbrock and Storey [10] and later investigated by Millman [12]:



where A_1 is the feed material, A_2 an intermediate, A_3 the desired product and A_4 the wasteful side product.

The rate constants, k_i , are given by

$$k_i = k'_i t_b \exp[-E_i(1/T - 1/658)] \tag{4-2}$$

$$i = 1, 2, \dots, 5$$

where k'_i is the frequency factor, t_b the total batch processing time, E_i the activation energy (divided by the gas constant) and T is the temperature.

For the kinetic parameters given in Table 4-1, the optimal temperature control policy to give a maximum concentration of A_3 has been studied when the reaction takes place in a plug-flow tubular reactor [10]. Millman considered batch reactor operation and compared the temperature schedules of optimal and proportional control policies for a fixed batch processing time t_b . Following Millman [12], the rate equations governing the state of the reaction are

$$r_1 = \frac{dx_1}{dt} = -(k_1 + k_2 + k_3) x_1 \quad (4-3)$$

$$r_2 = \frac{dx_2}{dt} = k_4(1-x_1-x_2-x_3) - k_5x_1 \quad (4-4)$$

$$r_3 = \frac{dx_3}{dt} = (k_2 + k_4) x_1 + k_5x_2 \quad (4-5)$$

with $0 \leq t \leq 1$

where time t is dimensionless due to normalization with the total batch processing time t_b , and x_1 , x_2 and x_3 are concentrations in moles per unit volume of A_1 , A_3 and A_4 respectively. The concentration of A_2 can be determined from the overall mass balance. The state variables are chosen to be A_1 , A_3 and A_4 since it is assumed in the numerical computations of Section 4.3 that noisy measurements of these variables are available.

TABLE 4-1

KINETIC PARAMETERS OF THE COMPLEX REACTION

<u>i</u>	<u>$k_i' t_b$</u>	<u>E_i ($^{\circ}\text{K}$)</u>
1	.077	8,000
2	.070	7,000
3	.029	7,500
4	.248	5,000
5	.006	7,500

4.2 Control Studies

4.2.1 Suboptimal Control Policy

It has been discussed in Chapter III that the optimal temperature control policy for a single reversible exothermic reaction taking place in a batch reactor is to have a maximum reaction rate at every instant. This situation will not, in general, result in a maximum yield of the desired product for complex reactions [11] and hence is not an optimal policy. Computational techniques such as Pontryagin's maximum principle, dynamic programming, hill climbing methods, etc. can be applied to calculate the optimal solution, providing it exists. However, since the required calculations are normally quite extensive and result in an "open-loop" control policy, updating the optimal control on-line to compensate for process parameter changes is generally not feasible. Consequently, only suboptimal control policies which can be adapted on-line will be investigated.

Two suboptimal control policies are discussed in this complex reaction example; one will be referred to as Millman's proportional control law and the other as the instantaneous performance index control law.

With all the kinetic parameters assumed to be known exactly as in Table 4-1, Millman [12] investigated a suboptimal control policy consisting of the following proportional control law:

$$T = K_1 + K_2 x_2 \quad (4-6)$$

and calculated the best values of $K_1 = 1120$ and $K_2 = 513$ through the use of a gradient method. (This control law was also considered in Section 3.2.3 for the single reaction.) His results [12] indicate that this suboptimal control resulted in yields which were very close to the optimal yields for several reaction examples.

A second type of suboptimal control policy can be derived by maximizing a performance index which depends only on the current values of the state variables. Several instantaneous performance index control schemes have been discussed by Weber and Lapidus [15]. Following Seinfeld [14] a suboptimal control policy will be derived by maximizing the instantaneous rate of reaction. The resulting control policy will be referred to here as the instantaneous performance index (IPI) control law.

Since A_3 is the desired product in this example, the suboptimal control policy based on maximizing the instantaneous rate of reaction of A_3 will be the solution of

$$\frac{\partial r_2}{\partial T} = 0 \quad (4-7)$$

Thus differentiating Equation (4-4) with respect to T , the temperature schedule is obtained as

$$T(t) = 1/\{\ln[\frac{E_5}{E_4} \frac{x_2}{(1-x_1-x_2-x_3)}]/(E_5-E_4) + 1/658\} \quad (4-8)$$

A comparison of the suboptimal and optimal control policies performing under "ideal conditions" is shown in Table 4-2. In the digital computer simulation it was assumed that the rate constants

TABLE 4-2

COMPARISON OF TEMPERATURE CONTROL POLICIES FOR THE COMPLEX REACTION

(850°K $\leq$ T $\leq$ 1120°K)

Time	Optimal Control [*]		Proportional Control [*]		IPI Control	
	Temp (°K)	Conc. of A ₃	Temp (°K)	Conc. of A ₃	Temp (°K)	Conc. of A ₃
0	1120	0	1120	0	1120	0
0.1	1120	0.126	1053	0.130	1120	0.126
0.2	1085	0.305	996	0.242	1120	0.299
0.3	994	0.372	961	0.310	1120	0.381
0.4	941	0.402	938	0.354	1120	0.414
0.5	909	0.419	923	0.385	961	0.423
0.6	888	0.430	911	0.406	885	0.427
0.7	873	0.437	904	0.421	850	0.429
0.8	864	0.442	898	0.432	850	0.430
0.9	857	0.446	895	0.440	850	0.430
1.0	852	0.448	891	0.445	850	0.430

* calculated values from reference [15]

were known and that noise free measurements of x_1 , x_2 and x_3 were available at a data sampling time, t_s , of 0.005. As in Millman's calculation of the optimal control policy [12], the temperature was constrained by, $850^\circ\text{K} \leq T \leq 1120^\circ\text{K}$. The results in Table 4-2 indicate that the suboptimal policies produce final concentrations of A_3 which are very close to the optimal value of 0.448.

4.2.2 Effect of Parameter Sensitivity on the Yield of A_3

Again it is assumed that the initial charge characteristics change unpredictably from batch to batch and can be represented by random variations in the activation energies, E_4 and E_5 . It is of interest to determine the effect of undetected changes in E_4 and E_5 on the final yield of A_3 .

In Table 4-3 yields are compared from the three control strategies when the actual kinetic parameters have changed by 20% from the nominal values in Table 4-1. The temperature control policies in Table 4-3 are based on the nominal parameter values. The "optimal control policy" in Table 4-3 was approximated by linear interpolation of the optimal temperature sequence calculated by Millman [12] and shown in Table 4-2.

It is found that the optimal temperature schedule based on the assumed activation energies does not always result in a higher yield than suboptimal control policies, when the activation energies change as in cases 1 and 2 of Table 4-3. One disastrous situation for the IPI control policy is case 3 where a yield of only 0.174 was obtained.

TABLE 4-3

EFFECT OF VARIATIONS IN E_4 AND E_5 ON THE FINAL YIELDS OF A_3

Case	Percent Variation in E_4	Percent Variation in E_5	Final Yield of A_3		
			Optimal [*]	Proportional [*]	IPI [*]
1	+20%	+20%	0.385	0.415	0.381
2	-20%	-20%	0.417	0.425	0.451
3	-20%	+20%	0.347	0.332	0.174
4	+20%	-20%	0.512	0.495	0.512

^{*}Control policy is based on the nominal values of E_4 and E_5 shown in Table 4-1

The effect of variations in the activation energies E_4 and E_5 on the control schemes has just been discussed. A similar situation occurs when inaccurate parameter values are used in the calculation of the control policy, i.e. suppose that the process parameters remain at the nominal values of Table 4-1, but the assumed model parameters differ. Table 4-4 shows the result of applying the IPI control law in this situation. Only in case 4, does the final yield differ significantly from the optimal yield of 0.448 or even the suboptimal yield of 0.430 obtained from the IPI control law when the activation energies are known exactly (cf. Table 4-2).

This type of comparison was not made for the proportional control and optimal control policies on account of the extensive programming effort that would be required to prepare the necessary computer programs.

4.3 Sequential State and Parameter Estimation

4.3.1 Open Loop Parameter Estimation

Suboptimal control policies with noise free measurements have been investigated in the previous section. It was found that Millman's proportional control law is not very sensitive to the variations in E_4 and E_5 . However, the required computations to find the best controller constants, K_1 and K_2 , for a given set of activation energies are extensive. The IPI control policy is quite sensitive when the assumed values of E_4 and E_5 used in the control calculations are too high and too low, respectively (as shown in cases 3 and 4 of Tables 4-3 and 4-4, respectively).

TABLE 4-4

EFFECT OF ERRORS IN THE ASSUMED VALUES OF E_4 AND E_5 USED IN THE IPI CONTROL LAW

Case	Percent Error in Assumed E_4^*	Percent Error in Assumed E_5^*	Final Yield of A_3
1	+20%	+20%	0.436
2	-20%	-20%	0.424
3	-20%	+20%	0.436
4	+15%	-15%	0.390

* Based on the nominal values of E_4 and E_5 shown in Table 4-1.

Hence on-line parameter estimation may be desirable to improve the final yield of A_3 by compensating for uncertain or changing parameters.

Assume no dynamic error is involved in the process and E_4 and E_5 are the only undetermined parameters. Again Detchmendi and Sridhar nonlinear filter technique [22] is applied to perform the on-line parameter (and state) estimation.

It is assumed that the measured values of the concentrations of A_1 , A_3 and A_4 contain random noise as described by the error model:

$$y_i = x_i[1 + \varepsilon_i(0, \sigma)], \quad i=1,2,3 \quad (4-9)$$

where y_i is the measured concentration of x_i and the noise error ε_i is assumed to be Gaussian distributed with zero mean and a standard deviation, σ .

Define state variables $\hat{x}_1(t)$, $\hat{x}_2(t)$ and $\hat{x}_3(t)$ as the corresponding estimated values of x_1 , x_2 and x_3 at time t . To reduce the "stiffness effect" in the filter equations (as in the simple reaction example), state variables corresponding to E_4 and E_5 are defined as $\hat{x}_4(t)$ and $\hat{x}_5(t)$ with

$$\hat{x}_4(t) = \frac{\hat{E}_4(t) - E_{4,ref}}{E_{4,ref}} \quad (4-10)$$

$$\hat{x}_5(t) = \frac{\hat{E}_5(t) - E_{5,ref}}{E_{5,ref}} \quad (4-11)$$

where $\hat{E}_4(t)$ and $\hat{E}_5(t)$ are the estimated values of E_4 , E_5 at any

instant t and $E_{4,ref}$, $E_{5,ref}$ are fixed reference values.

Then the filter equations (2-7 to 2-9) can be developed with the state equations and Jacobian as

$$f_1 = -(k_1 + k_2 + k_3) \hat{x}_1 \quad (4-12)$$

$$f_2 = \hat{k}_4(1 - \hat{x}_1 - \hat{x}_2 - \hat{x}_3) - \hat{k}_5 \hat{x}_2 \quad (4-13)$$

$$f_3 = (k_2 + \hat{k}_4) \hat{x}_1 + \hat{k}_5 \hat{x}_2 \quad (4-14)$$

$$f_4 = 0 \quad (4-15)$$

$$f_5 = 0 \quad (4-16)$$

$$f_{11} = -(k_1 + k_2 + k_3) \quad (4-17)$$

$$f_{12} = 0 \quad (4-18)$$

$$f_{13} = 0 \quad (4-19)$$

$$f_{14} = 0 \quad (4-20)$$

$$f_{15} = 0 \quad (4-21)$$

$$f_{21} = -\hat{k}_4 \quad (4-22)$$

$$f_{22} = -\hat{k}_4 - \hat{k}_5 \quad (4-23)$$

$$f_{23} = -\hat{k}_4 \quad (4-24)$$

$$f_{24} = (1 - \hat{x}_1 - \hat{x}_2 - \hat{x}_3) \hat{k}_4 [-E_{4,ref}(1/T - 1/658)] \quad (4-25)$$

$$f_{25} = -\hat{x}_2 \hat{k}_5 [-E_{5,ref}(1/T - 1/658)] \quad (4-26)$$

$$f_{31} = k_2 + \hat{k}_4 \quad (4-27)$$

$$f_{32} = \hat{k}_5 \quad (4-28)$$

$$f_{33} = 0 \quad (4-29)$$

$$f_{34} = \hat{x}_1 \hat{k}_4 [-E_{4,\text{ref}} (1/T - 1/658)] \quad (4-30)$$

$$f_{35} = \hat{x}_2 \hat{k}_5 [-E_{5,\text{ref}} (1/T - 1/658)] \quad (4-31)$$

$$f_{41} = f_{42} = f_{43} = f_{44} = f_{45} = 0 \quad (4-32)$$

$$f_{51} = f_{52} = f_{53} = f_{54} = f_{55} = 0 \quad (4-33)$$

with the relations

$$\hat{k}_4 = (k_4' t_b) \exp [-(E_{4,\text{ref}} + \hat{x}_4 E_{4,\text{ref}})(1/T - 1/658)] \quad (4-34)$$

$$\hat{k}_5 = (k_5' t_b) \exp [-(E_{5,\text{ref}} + \hat{x}_5 E_{5,\text{ref}})(1/T - 1/658)] \quad (4-35)$$

Suppose the reactor state is known initially and the reference values of $E_{4,\text{ref}}$ and $E_{5,\text{ref}}$ are chosen to be the initially assumed values of E_4 and E_5 . Then the initial conditions of the filter equations are,

$$\hat{x}_1(0) = 1$$

$$\hat{x}_2(0) = \hat{x}_3(0) = \hat{x}_4(0) = \hat{x}_5(0) = 0$$

irrespective of the assumed values of E_4 and E_5 .

For this investigation of the nonlinear filters under open loop conditions, it will be assumed that the reactor temperature

varies linearly with time:

(obtained from a linear approximation to the optimal temperature schedule of Table 4-2)

$$T = 1120 - 250 t \quad (4-36)$$

As in Section 3.3.1 numerical experimentation was required to find a satisfactory initial covariance matrix $\underline{\underline{P}}(0)$. From the experience of finding $\underline{\underline{P}}(0)$ in Section 3.3.1 for the single reactor, a diagonal matrix of $\underline{\underline{P}}(0)$ was first tested with the elements corresponding to parameters larger than the elements corresponding to the state variables. A slow convergent rate of filter estimation resulted using a diagonal matrices for $\underline{\underline{P}}(0)$. To improve the rate of convergence, the off-diagonal elements of $\underline{\underline{P}}(0)$ were also tested. After 20 trial runs, the following initial covariance matrix $\underline{\underline{P}}(0)$ was found to be satisfactory.

$$\underline{\underline{P}}(0) = \begin{bmatrix} 0.5 & 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 250 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 & 250 \end{bmatrix}$$

As discussed in Section 2.2, the weighting matrices in the performance index must also be specified. Since dynamic errors are not considered in this complex batch reaction, only the weighting matrix, $\underline{\underline{Q}}(t)$, must be specified. For this example, the following matrix

$$\underline{\underline{Q}}(t) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{with } 0 \leq t \leq 1$$

was arbitrarily chosen to place identical weight on each measured concentration.

With all the initial conditions available, the filter equations were integrated by a Runge-Kutta-Gill 4-th order routine [43] with the integration interval equal to the data sampling interval of $t_s = 0.005$. The simulated process data were generated by integrating Equations (4-3) to (4-5) with the same integration routine and the measured concentrations calculated from Equation (4-9) using unbiased Gaussian distributed random numbers with a standard deviation of $\sigma = 0.1$ and zero mean. For the piecewise recursive filter algorithm, $t_p = 0.01$ was used, i.e. the updating interval of the covariance differential matrix was twice the sampling interval. As in Chapter III, the original filter algorithm will be referred to as Filter I and the piecewise recursive filter algorithm as Filter II. The filter estimates are shown in Figures 4-1 and 4-2 for 20% errors in the initial guesses of E_4 and E_5 . The solid and dashed lines correspond to cases 1 and 2 respectively of Table 4-4.

The results in Figure 4-1 and 4-2 indicate that the estimates of E_4 converge quite rapidly for both filters while the estimates of E_5 converge slowly for both filters in case 2 where the initial guess of E_5 is 20% low. For the initial guesses of E_4 and E_5 corresponding to cases 3 and 4 of Table 4-4, the results are quite similar to

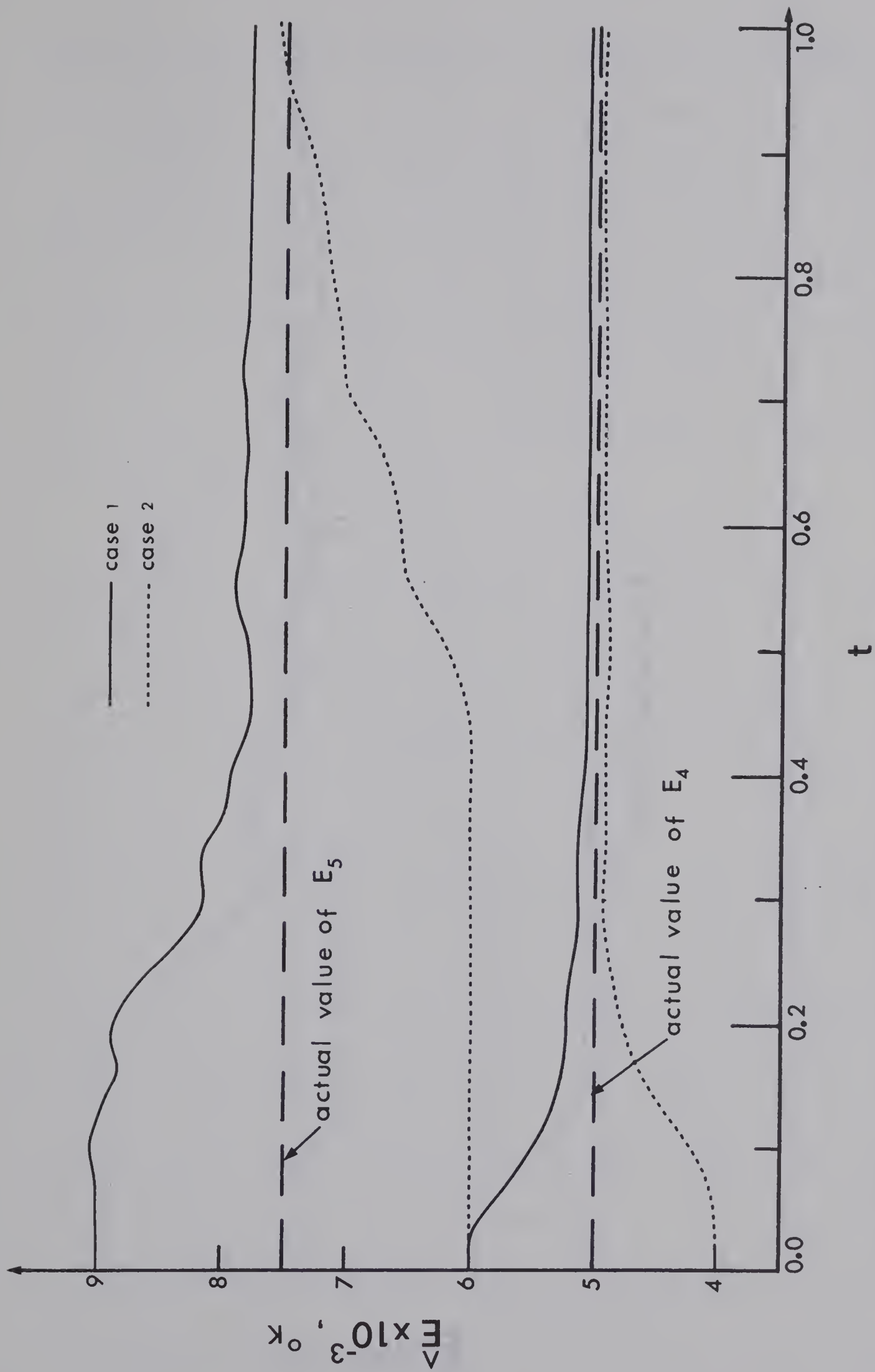


Figure 4-1 Open Loop Estimation of E_4 and E_5 by Filter I ($t_s = 0.005$, $\sigma = 0.1$)

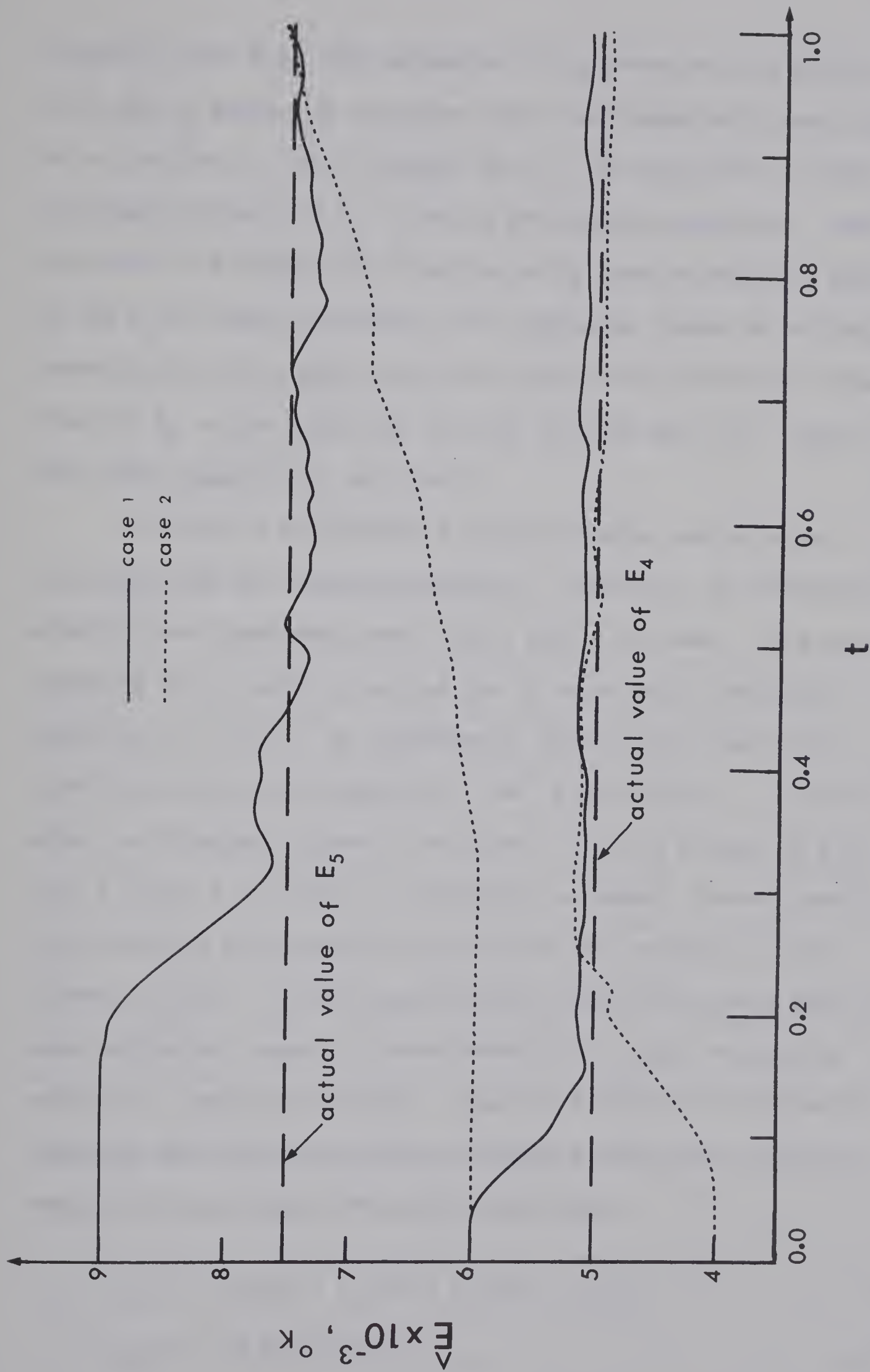


Figure 4-2 Open Loop Estimation of E_4 and E_5 by Filter II ($t_s = 0.005$, $\sigma = 0.1$, $t_p = 2t_s$)

Figures 4-1 and 4-2. The estimation of E_4 converges very quickly, while the E_5 estimation converges very slowly especially when -20% error involved in initial guesses of E_5 . The reason for a slowly convergent estimate of E_5 is due to the reaction mechanism. When the reaction first begins, the formation of A_4 from the reaction path of k_2 and k_3 as shown in Equation (4-1) dominates, hence the estimated concentration of A_4 does not differ greatly from the actual concentrations of A_4 in the beginning, thus the driving term, $[\underline{y} - \underline{h}(\hat{\underline{x}}, t)]$, in the filter equations is very small.

In Filter I estimation, 5 state variables are estimated (including the two unknown parameters). Therefore, 20 differential equations are integrated every time a sample is taken. If algebraic equations can be used to replace the 15 covariance differential equations of Filter I, as suggested by Seinfeld and Chen [14], a significant saving in computation time is predictable. In order to obtain satisfactory algebraic equations, the time history of $\underline{\underline{P}}(t)$ from a Filter I or Filter II simulation is needed, then exponential approximations are assumed to approximate the response of each element of $\underline{\underline{P}}(t)$. If these approximate expressions provide poor parameter estimates, numerical experimentation is again required to modify the algebraic equations. About 10 trials were required to determine the following algebraic equations which were chosen to replace the covariance differential equations.

$$P_{11}(t) = P_{12}(t) = P_{13}(t) = P_{14}(t) = P_{15}(t) = 0 \quad (4-36)$$

$$P_{22}(t) = 19.8 \exp(-3.3t) \quad (4-37)$$

$$P_{23}(t) = -3.4 \exp(-1.5t) \quad (4-38)$$

$$P_{24}(t) = 117 \exp(-8.8t) \quad (4-39)$$

$$P_{25}(t) = -17.8 \exp(-1.21t) \quad (4-40)$$

$$P_{33}(t) = 9.8 \exp(-2.1t) \quad (4-41)$$

$$P_{34}(t) = 8.2 \exp(-1.44t) \quad (4-42)$$

$$P_{35}(t) = 47.6 \exp(-1.85t) \quad (4-43)$$

$$P_{44}(t) = 270 \exp(-3.0t) \quad (4-44)$$

$$P_{45}(t) = 43.8 \exp(-3.7t) \quad (4-45)$$

$$P_{55}(t) = 533 \exp(-4.7t) \quad (4-46)$$

The filter obtained by replacing the elements of $\underline{P}(t)$ with algebraic equations will be referred to as the Filter III algorithm. Figure 4-3 shows the estimation provided by Filter III with initial guesses of E_4 and E_5 corresponding to cases 1 and 2 of Table 4-4. By comparison with the Figures 4-1 and 4-2, the Filter III algorithm seems to be a feasible approach to perform unknown parameter estimation. The same situation in the fast convergence of $\hat{E}_4$ is quite predictable, since the algebraic equations are chosen to approximate the time history of the covariance matrix elements of Filters I and II.

4.3.2 Comparison of Computation Times for Filters I, II and III

In order to get a rough idea about how much computation time can be saved by using the simplified nonlinear filter algorithms, object decks for Filter I, II and III were generated to perform the computation on an IBM 360/67 computer with the MTS operating system.

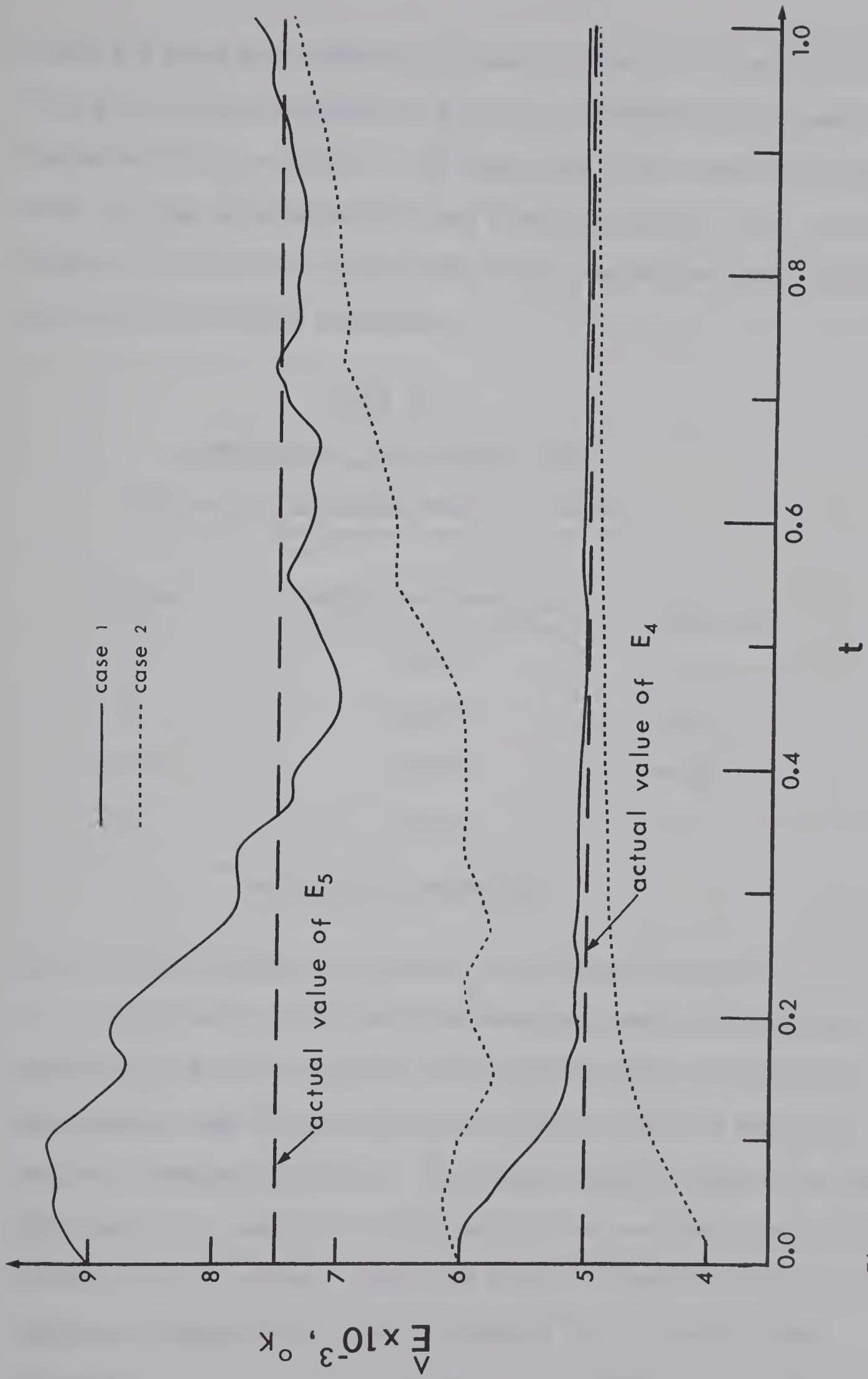


Figure 4-3 Open Loop Estimation of E_4 and E_5 by Filter III ($t_s = 0.005$, $\sigma = 0.1$)

Table 4-5 gives the computer CPU time of Filter I, II and III estimation with initial estimates of E_4 and E_5 corresponding to case 1 of Table 4-4 and $t_s = 0.005$. It is found that a 25% reduction in computation time can be obtained by using Filter II with $t_p = 2 t_s$, while the Filter III algorithm can save 40% of the computation time in comparison with the Filter I estimation.

TABLE 4-5
COMPARISON OF COMPUTATION TIMES
FOR THE FILTER ALGORITHMS ($t_s = 0.005$)

<u>Filter</u>	<u>Computation Time* (sec)</u>	<u>t_p</u>
I	21.8	-
II	16.3	$2 t_s$
II	13.8	$4 t_s$
III	12.2	-

* includes I/O operations

4.3.3 Effect of Sampling Interval on Parameter Estimation

Since most of the real-time computers used in the process industries are small or medium size computers, the computational requirements made of the computer is another important aspect of on-line parameter estimation. If a large sampling time can be used, the load on the computer for data acquisition and the filter calculations will be reduced. Hence the effect of sampling interval on parameter estimation will be investigated for all three filter algorithms. For $t_s = 0.01$, the resulting parameter estimates showed

essentially the same convergence as indicated in Figures 4-1 to 4-3 for $t_s = 0.005$. As a further check, $t_s = 0.02$ was investigated for all three filters with $t_p = 2 t_s$ being used for the Filter II estimation. Figure 4-4 shows typical results for the case 1 initial conditions of Table 4-4. All filters provide a rapidly converging estimate of E_4 , while the estimation of E_5 is poor for Filters I and III, but Filter II still gives a reasonable estimation. When t_s was increased to a value of 0.04, all three filters gave poor estimates of E_4 and E_5 .

4.3.4 Effect of t_p on Filter II Estimation

To investigate the effect of t_p on Filter II estimation, values of $t_s = 0.005$ and $t_p = 0.02$ (i.e. $t_p = 4 t_s$) were used in the simulation. For the initial parameter estimates of $\hat{E}_4(0)$ and $\hat{E}_5(0)$ corresponding to cases 1 and 2 of Table 4-4, Figure 4-5 shows the Filter II estimation with $t_p = 4 t_s$. It is found that the parameter estimates are poor even for E_4 . By comparison, in the last section, when $t_s = 0.02$ and $t_p = 0.04$ (i.e. $t_p = 2 t_s$) were used in the Filter II estimation, good estimates of E_4 and E_5 were obtained. Hence in the actual application of the Filter II algorithm, the relation of $t_p = 2t_s$ appears desirable in this example in order to obtain satisfactory estimates. Despite this restriction on t_p , a significant reduction in computer time is achieved by Filter II as shown in Table 4-5.

4.3.5 Parameter Estimation When Some States are not Measured

In the above calculations, the state knowledge required in

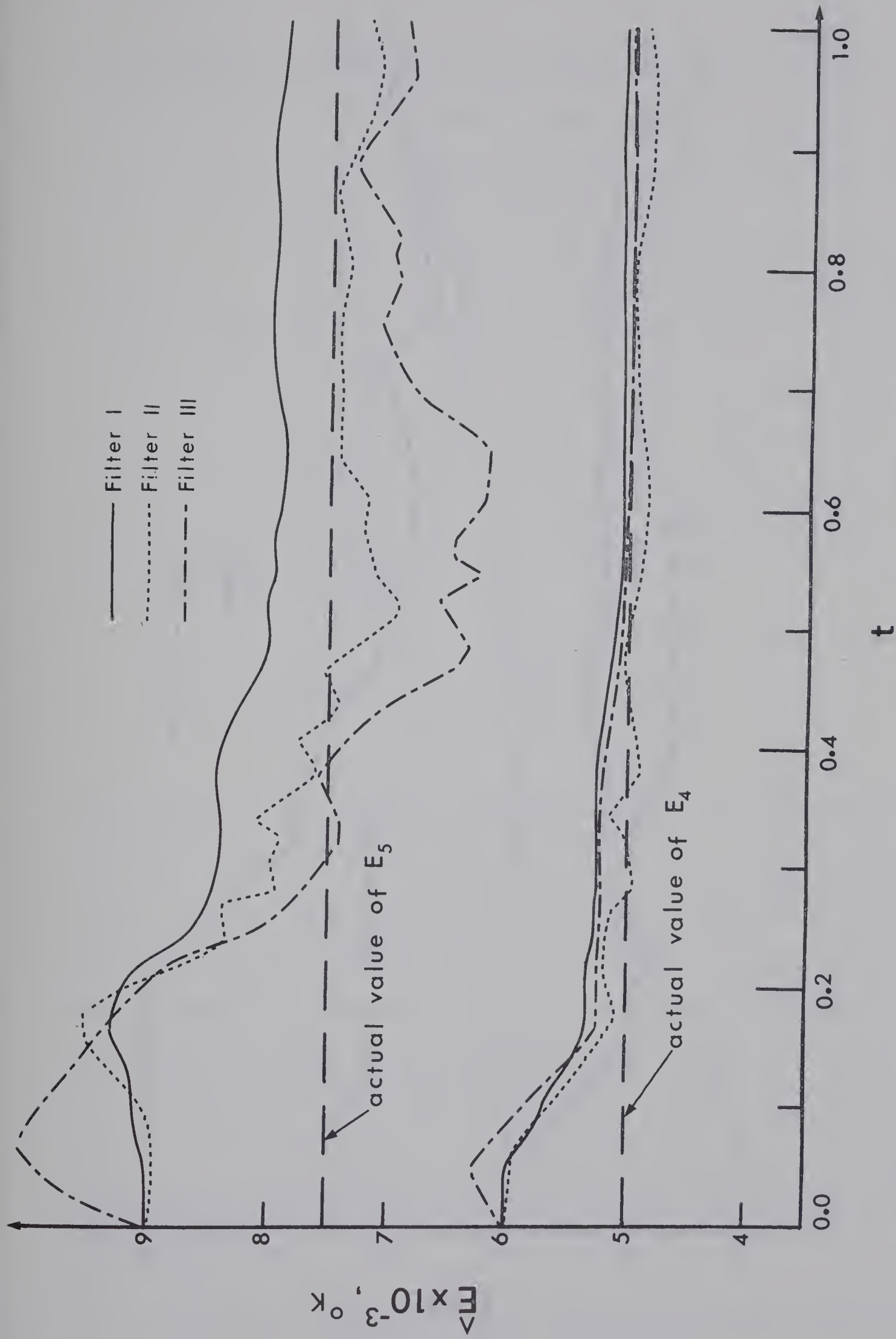


Figure 4-4 Open Loop Estimation of E_4 and E_5 by the Three Filters (case 1, $t_s = 0.02$, $\sigma = 0.1$)

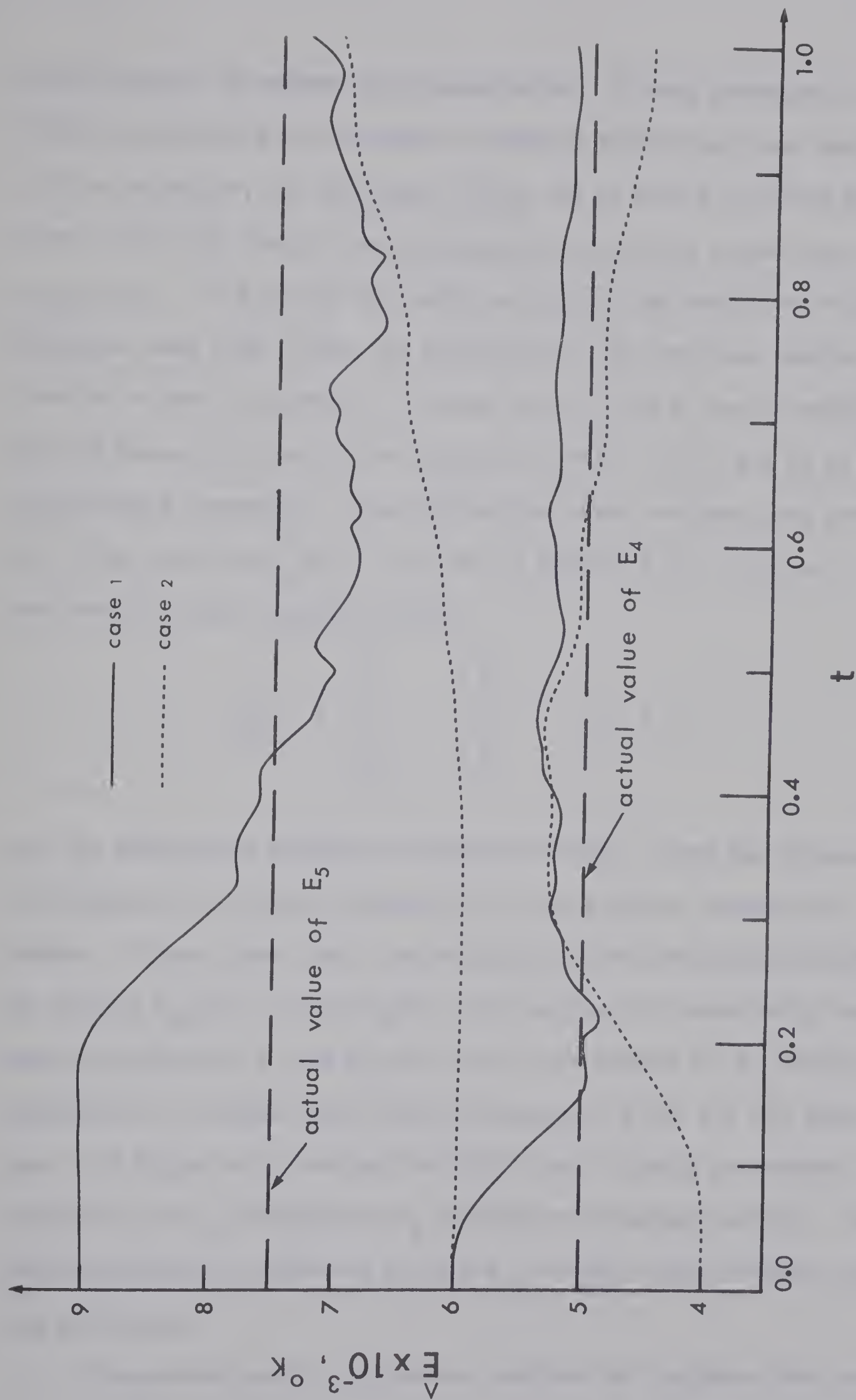


Figure 4-5 Effect of t_p on Filter II Estimation ($t_s = 0.005$, $t_p = 4t_s$)

control policy is assumed to be measurable. In many processes, it is either not possible or practical to measure all of the state variables. In this situation, the nonlinear filter can be used to provide estimates of all the states from measurement data of the states which are accessible. To evaluate the applicability of the nonlinear filter technique when some states are inaccessible, the previous complex reaction scheme is examined. Suppose only A_1 and A_3 can be measured and the measured states follow Equation (4-4). Let E_4 and E_5 be the undetermined parameters. Then define the state variables and develop the filter equations (2-7 to 2-9) as in Section 4.3.1 with the arbitrarily chosen weighting matrix

$$\underline{\underline{Q}}(t) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad 0 \leq t \leq 1$$

and the temperature schedule in Equation (4-36). Then the process is simulated on the digital computer as in the previous computation scheme. It was found that a modification of the previously used $\underline{\underline{P}}(0)$ by setting $P_{44}(0) = 50$ and $P_{55}(0) = 75$ resulted in essentially the same estimation of E_1 and E_5 as in case 1 of Figure 4-1 by Filter I estimation. But when the initial estimates of state are the same as case 2 of Figure 4-1, the modified $\underline{\underline{P}}(0)$ gave a slowly convergent estimation of E_5 although the E_4 estimation converged rapidly. Further experimentation by adjusting P_{44} and P_{55} in $\underline{\underline{P}}(0)$ could probably improve the estimation.

Hence when certain states are required to implement the control

policy but are not measured, the nonlinear filter technique is a feasible way to supply the required state estimates.

4.3.6 Closed Loop Parameter Estimation

In Chapter III, the parameter estimation and optimal cooling paths could be separated since the parameter estimation was essentially completed during adiabatic operation (i.e. before the switching point for optimal cooling was reached). In this complex reaction example, parameter estimation could in principle be performed during isothermal operation or some other specified temperature schedule and then a switch made to a different control strategy after the parameter estimation converges. Unfortunately, the previous open loop calculations indicated that the estimation of E_5 inherently involve slow convergence. An alternative control strategy proposed by Seinfeld [14,38] is to use feedback control with a nonlinear filter added to the control loop. In this case the parameter estimation and control action are performed simultaneously. The block diagram for the proposed control scheme is shown in Figure 4-6. Where $\varepsilon(t)$ is the observation noise and the controller can be any suboptimal controller. Note that the suboptimal control is based on the estimate of the state supplied by the filter rather than the noisy measurements.

This control strategy is simulated in the complex reaction example with the IPI control policy chosen as the suboptimal control policy. Assume no dynamic errors are involved in the process and the initial state of the reactor is known exactly. Then with the same initial covariance matrix $\underline{\underline{P}}(0)$ and weighting matrix $\underline{\underline{Q}}(t)$ that were used

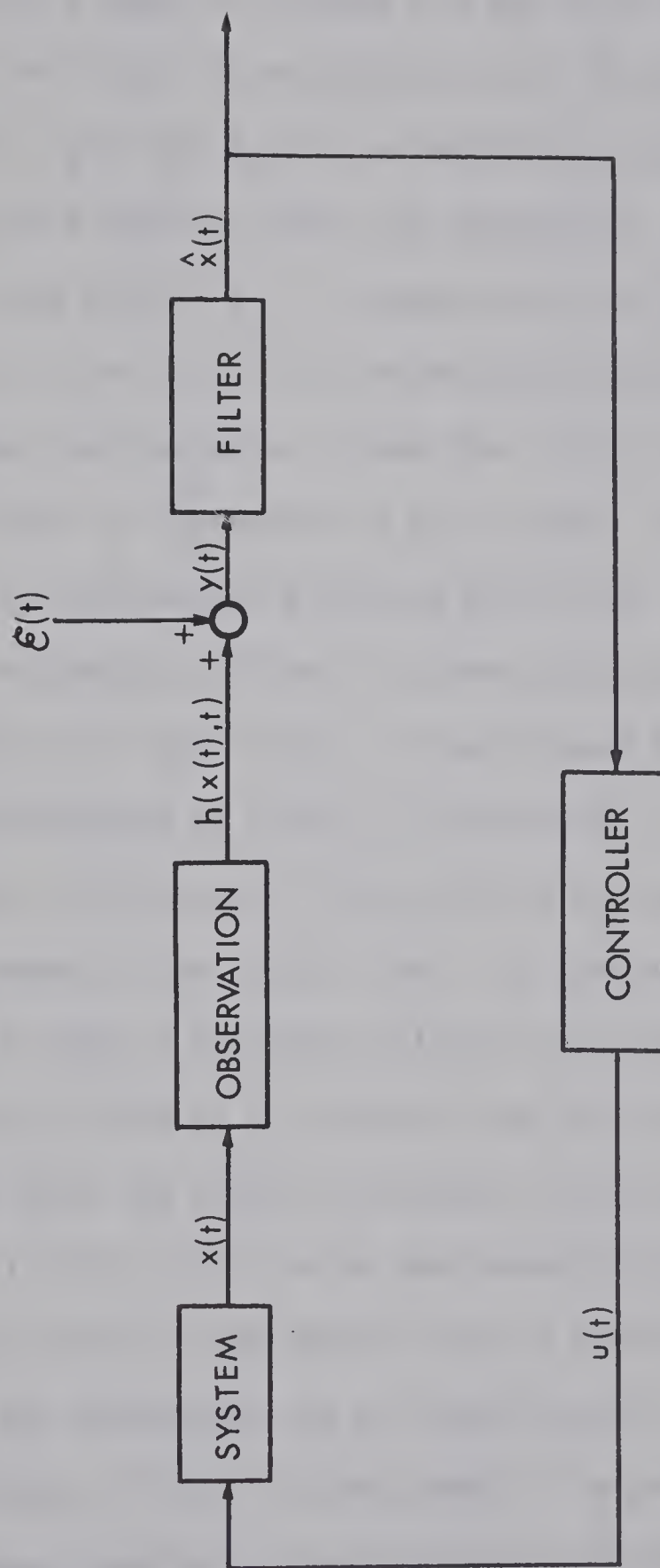


Figure 4-6 Block Diagram of Feedback Control with Filter Added [14, 38]

in the open loop estimation, the closed loop system is simulated. Filter I estimations are shown in Figures 4-7 and 4-8, Filter II estimations are shown in Figures 4-9 and 4-10, and Figures 4-11 and 4-12 show the Filter III estimations with initial estimates of E_4 and E_5 (i.e. $\hat{E}_4(0)$ and $\hat{E}_5(0)$) corresponding to the 4 cases in Table 4-4. As in the previous open loop estimation, convergence of $\hat{E}_5$ is slower than that of $\hat{E}_4$. In comparison with the previous open loop estimation, Filter I and III provide better parameter estimates during close loop operation. When the initial estimate of E_5 is low, the Filter II estimation of E_5 is poor. The Filter II estimation could be improved by selecting $\underline{P}(0)$ so as to give satisfactory parameter estimates by Filter II during closed loop operation. As noted earlier, all the Filter II results used the $\underline{P}(0)$ selected for open loop estimation by Filter I (see Section 4.3.1).

Table 4-6 gives the final yield of A_3 when the nonlinear filter is added to the control loop. In comparison with the results of Table 4-4 where a nonlinear filter is not used, the addition of the nonlinear filter in the control loop only small changes for cases 1 - 3. But when the initial estimates of E_4 and E_5 corresponded to case 4 of Table 4-4, a large improvement in the final yield of A_3 was obtained when the nonlinear filter is added to the control loop. Hence when the parameters are not known exactly, closed loop control with a nonlinear filter included seems to be practical.

Another problem as shown in Table 4-3 occurs when the values of E_4 and E_5 change (e.g. due to catalyst decay) as in case 3. Here the IPI control policy gives a very poor final yield of A_3 if parameter

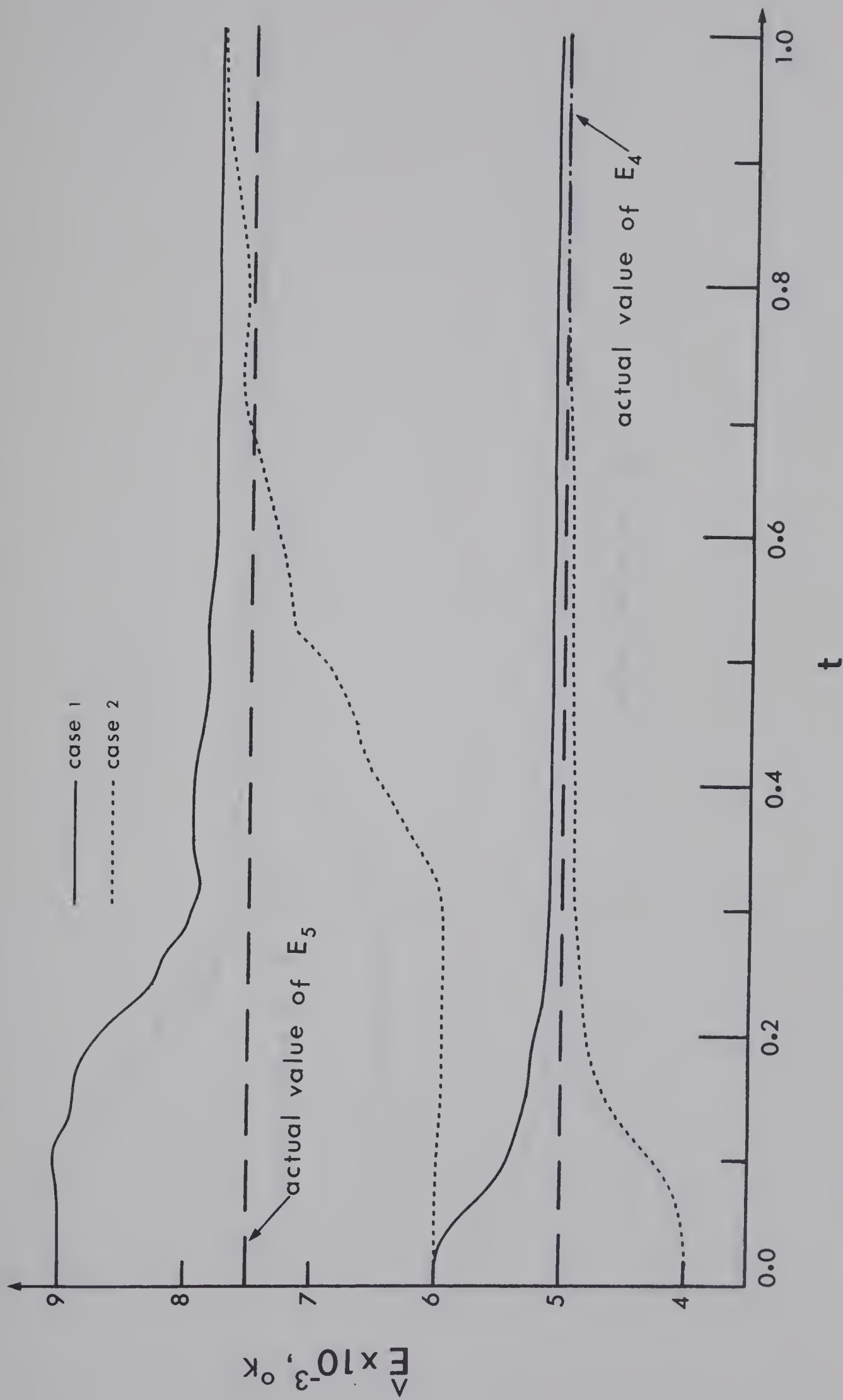


Figure 4-7 Closed Loop Estimation of E_4 and E_5 by Filter I for Cases 1 and 2

($t_s = 0.005$, $\sigma = 0.1$)

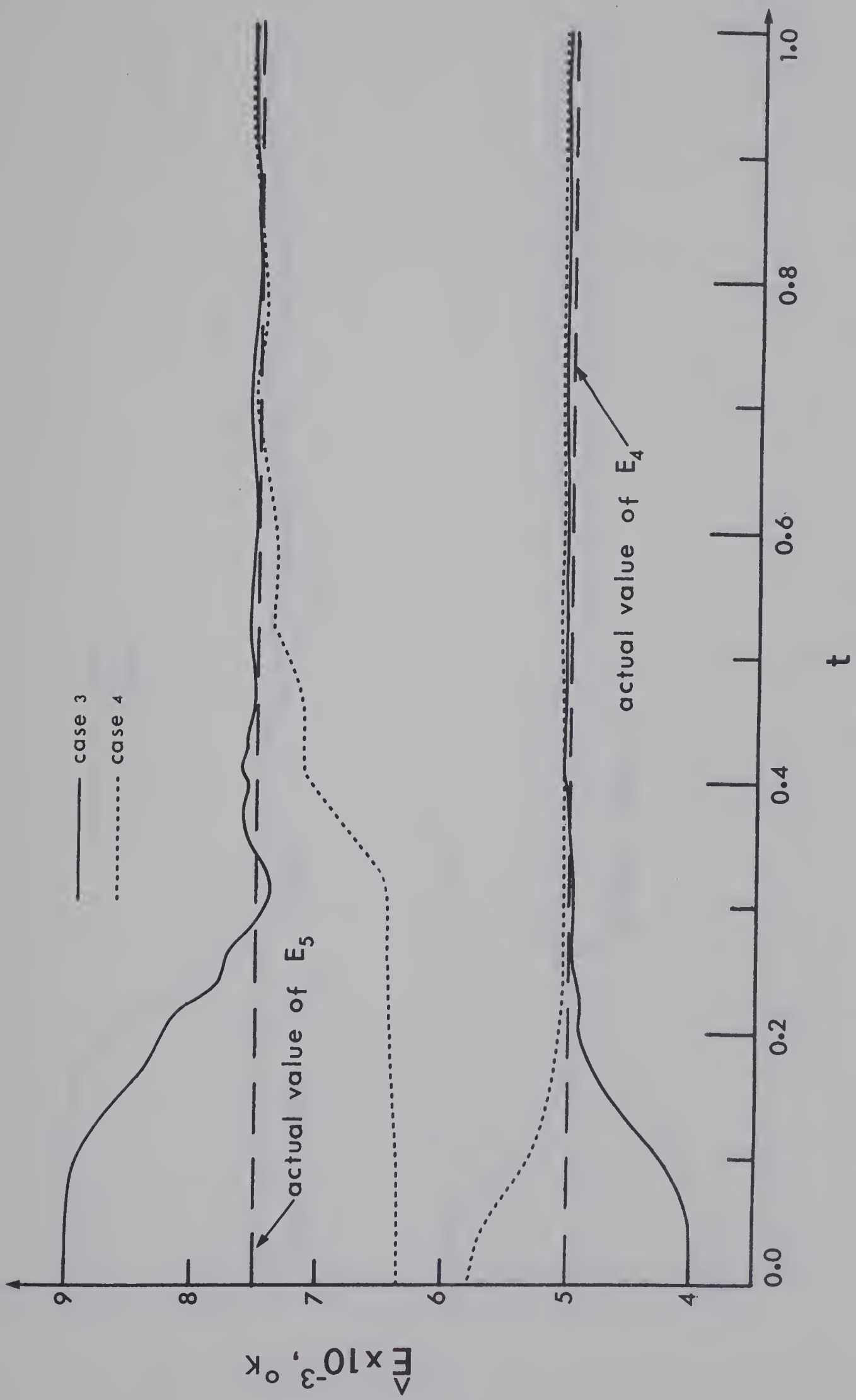


Figure 4-8 Closed Loop Estimation of E_4 and E_5 by Filter I for Cases 3 and 4
 ($t_s = 0.005, \sigma = 0.1$)

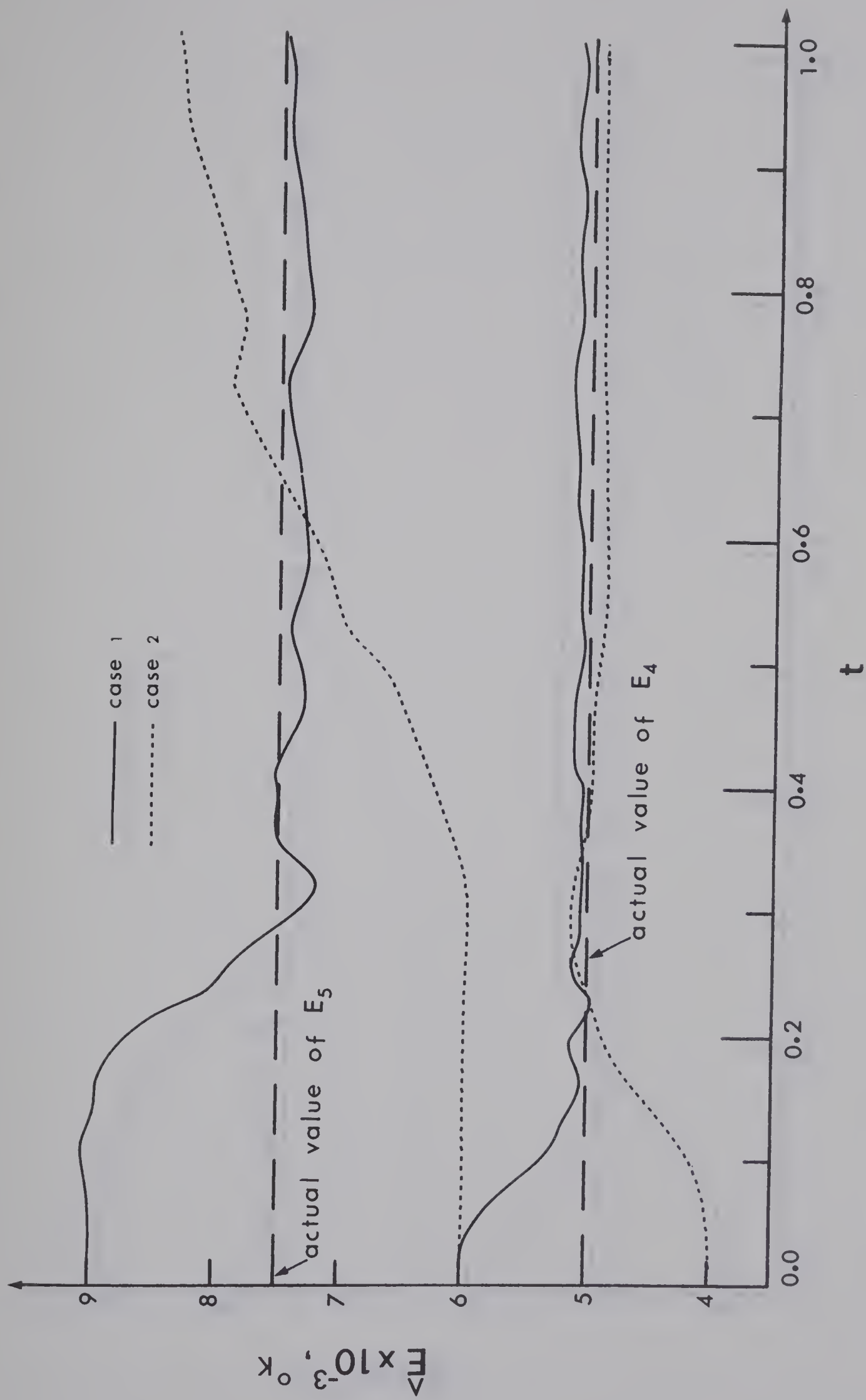


Figure 4-9 Closed Loop Estimation of E_4 and E_5 by Filter II for Cases 1 and 2

($t_s = 0.005$, $\sigma = 0.1$, $t_p = 2t_s$)

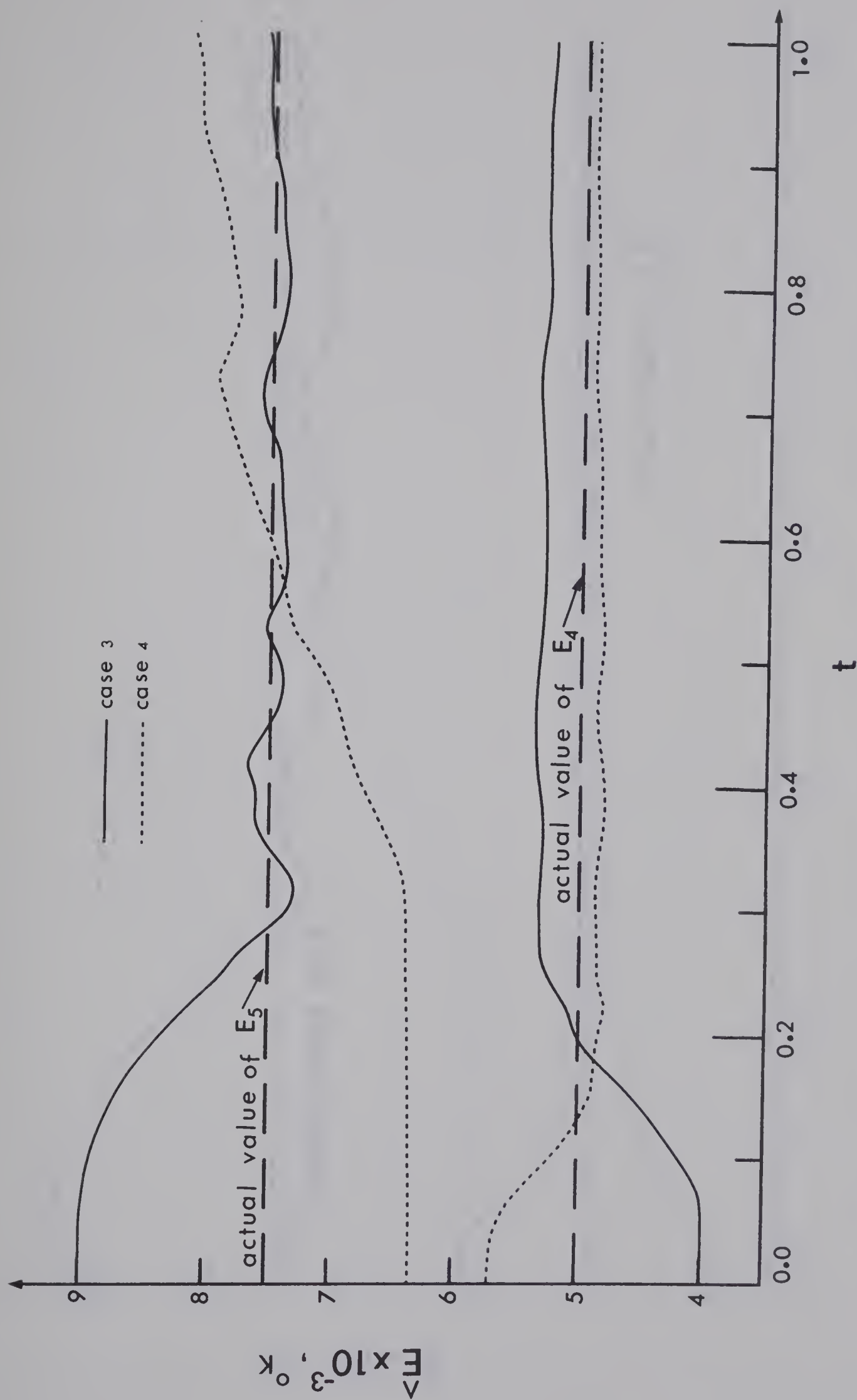


Figure 4-10 Closed Loop Estimation of E_4 and E_5 by Filter II for Cases 3 and 4

($t_s = 0.005$, $\sigma = 0.1$, $t_p = 2t_s$)

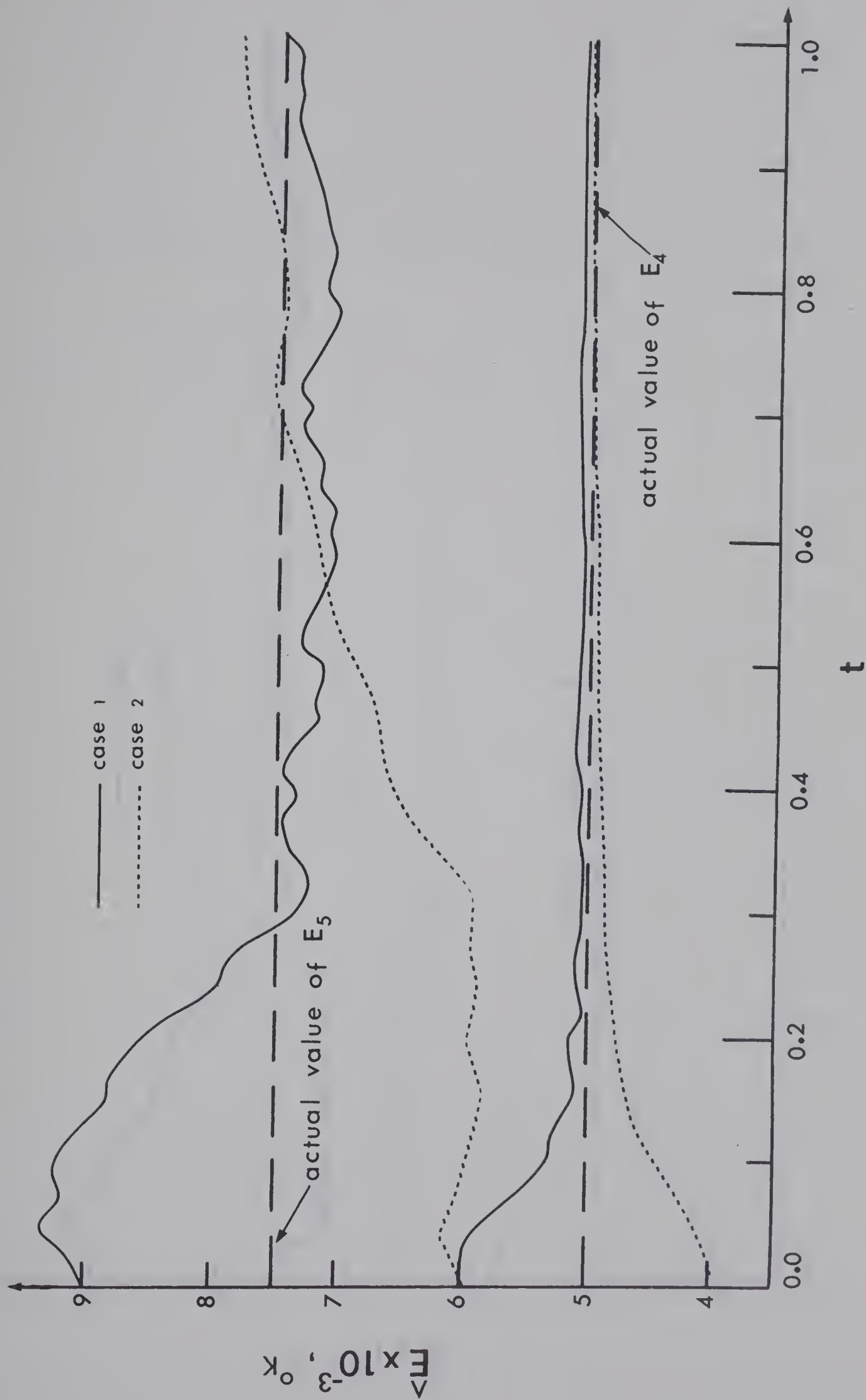


Figure 4-11 Closed Loop Estimation of E_4 and E_5 by Filter III for Cases 1 and 2
 ($t_s = 0.005$, $\sigma = 0.1$)

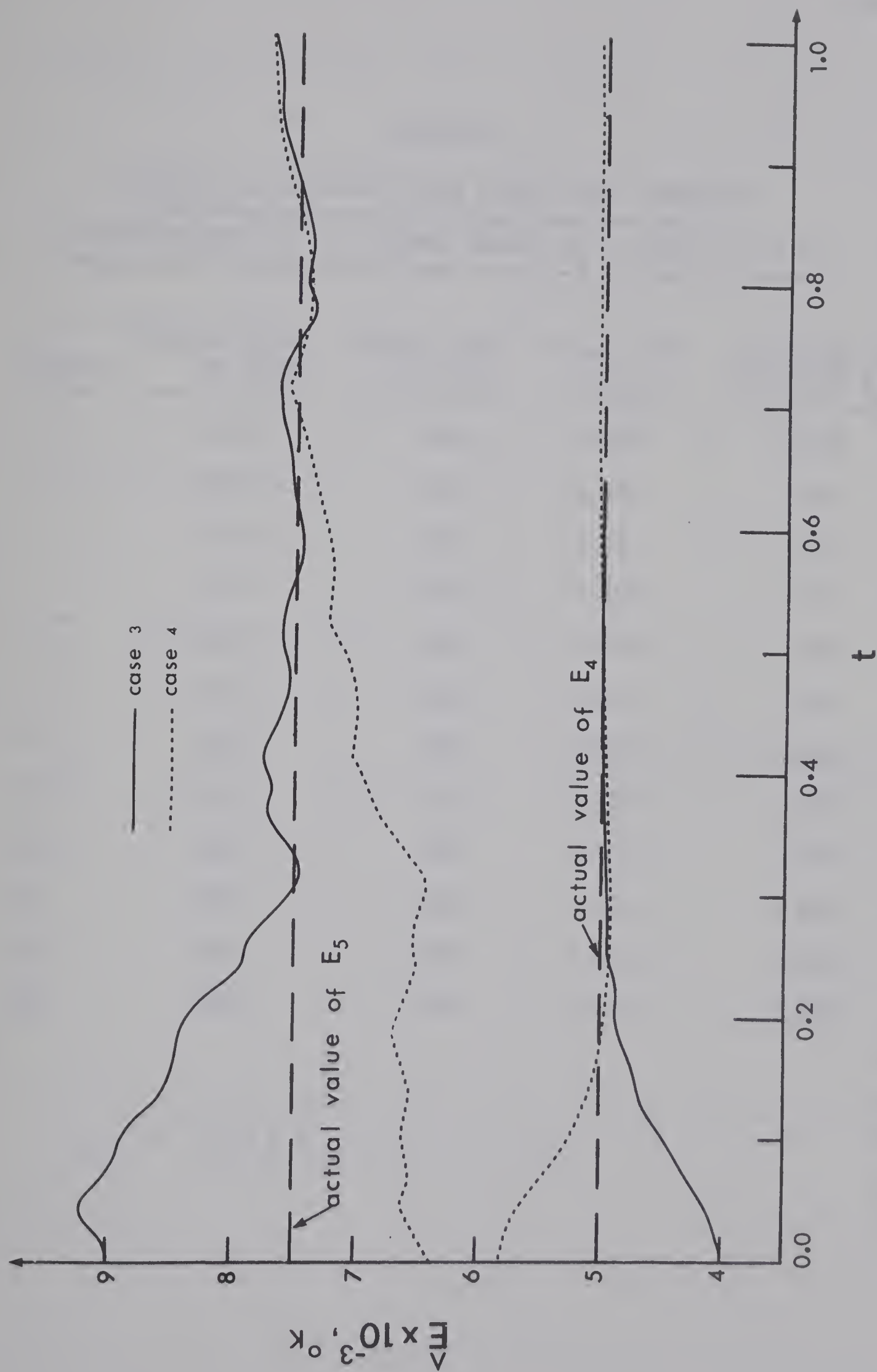


Figure 4-12 Closed Loop Estimation of E_4 and E_5 by Filter III for Cases 3 and 4

($t_s = 0.005$, $\sigma = 0.1$)

TABLE 4-6

YIELDS OF A_3 OBTAINED USING CLOSED LOOP PARAMETER
 ESTIMATION AND THE IPI CONTROL POLICY ($t_s = 0.005$, $\sigma = 0.1$)

Filter	Percent Error in $\hat{E}_4(0)$	Percent Error in $\hat{E}_5(0)$	Final Yield of A_3	Estimated Final Yield of A_3
I	+20%	+20%	0.437	0.435
I	-20%	-20%	0.422	0.426
I	-20%	+20%	0.431	0.431
I	+15%	-15%	0.428	0.431
II*	+20%	+20%	0.432	0.431
II*	-20%	-20%	0.420	0.421
II*	-20%	+20%	0.432	0.432
II*	+15%	-15%	0.425	0.427
III	+20%	+20%	0.432	0.430
III	-20%	-20%	0.421	0.426
III	-20%	+20%	0.434	0.433
III	+15%	-15%	0.426	0.429

$$* \quad t_p = 2 \quad t_s$$

estimation is not performed. Table 4-7 compares the final yields of A_3 and estimates of E_4 and E_5 when a filter is added and when no filter is used. The corresponding concentration histories of A_3 are shown in Figure 4-13. The estimated concentration of A_3 is not shown in Figure 4-13, since the estimated values are quite close to the actual concentrations. Figure 4-14 shows the Filter I estimation of E_4 and E_5 . Thus again it has been demonstrated that a nonlinear filter can be used to "track" sensitive parameters during batch reactor operation and give improved control.

TABLE 4-7
EFFECT OF VARIATIONS IN E_4 AND E_5 ON FINAL YIELD
OF A_3 (IPI CONTROL POLICY, $t_s = 0.005$, $\sigma = 0.1$)

Filter	Final Yield of A_3	Estimated Final Yield of A_3	Final Parameter Estimates [*]	
			Percent Error in E_4	Percent Error in E_5
None	0.173	-	-20%	+20%
I	0.322	0.325	+2.4%	+2.1%
II ^{**}	0.324	0.319	-1.0%	+9.6%
III	0.321	0.322	+1.6%	+5.0%

* Initial parameter estimates were chosen to be the nominal parameter values (i.e. $\hat{E}_4(0) = 5000$, $\hat{E}_5(0) = 7500$)

** $t_p = 2 t_s$

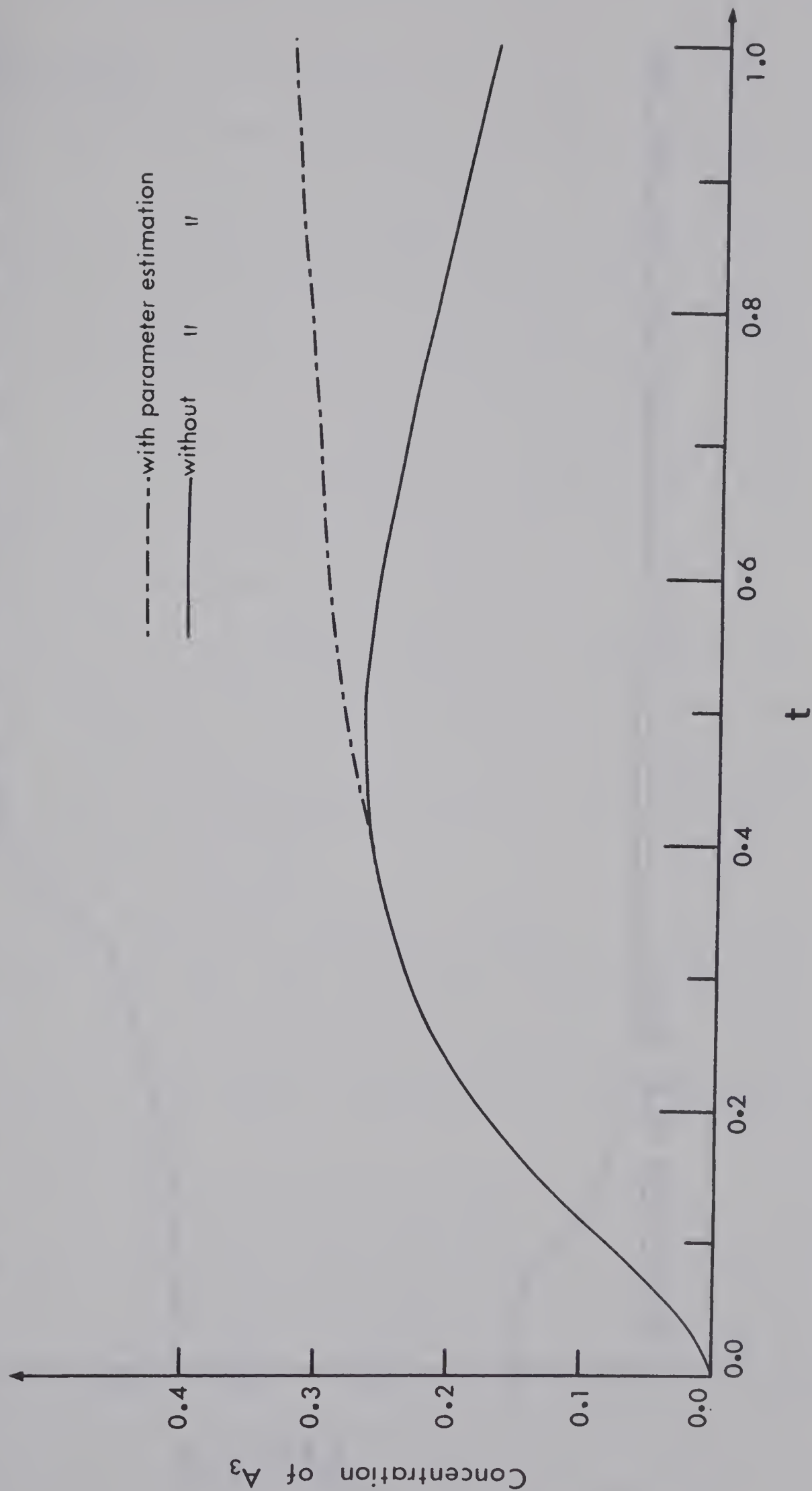


Figure 4-13 Yield of A_3 When IPI Control Policy is Used Both With Parameter Estimation and Without Parameter Estimation

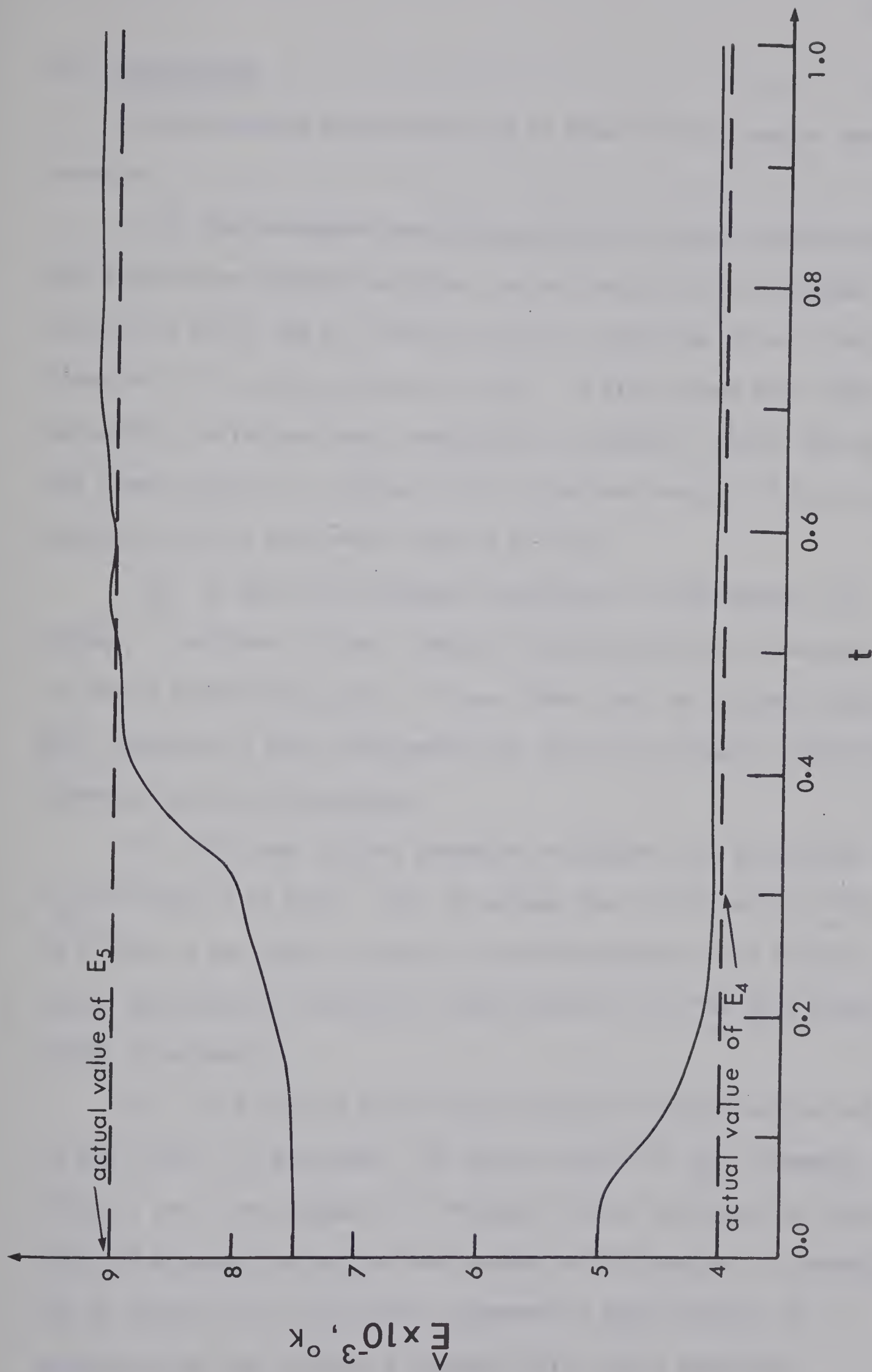


Figure 4-14 IPI Control Scheme with Filter I Added in the Feedback Loop to Estimate

E_4 and E_5 ($t_s = 0.005$, $\sigma = 0.1$)

4.4 Conclusions

The following conclusions can be made for the complex reaction example.

(1) The parameter sensitivity analysis showed that the optimal and proportional control policies are not sensitive to parameter variations while the IPI control policy is sensitive to only one combination of E_4 and E_5 values (case 3). It also showed that when the parameters varied and were undetected, the optimal control policy did not always result in a higher yield of desired product of A_3 in comparison with the suboptimal control policies.

(2) In open loop parameter estimation by Detchmندی and Sridhar nonlinear filter, numerical experimentation is required to find a satisfactory $\underline{\underline{P}}(0)$. It was found that the diagonal matrix $\underline{\underline{P}}(0)$ resulted in slow convergence but the use of nonzero off-diagonal elements improved convergence.

(3) For some initial parameter estimates, the estimation of E_5 by Filter II is poor. This is because the initial matrix $\underline{\underline{P}}(0)$ used in Filter II was based on numerical experimentation with Filter I. In actual applications, numerical experimentation to find $\underline{\underline{P}}(0)$ should use Filter II directly.

(4) In finding a satisfactory algebraic approximation for $\underline{\underline{P}}(0)$ in the Filter III algorithm, the time variation of $\underline{\underline{P}}(t)$ elements of Filter I or II are needed for different initial estimates of state. Since 15 algebraic equations are needed in the example, a systematic way of finding the satisfactory exponential approximation is to determine the most sensitive elements first, then numerical

experimentation can be performed on the sensitive elements to find satisfactory expressions.

(5) Closed loop scheme of performing parameter estimation and control action simultaneously seems to be a feasible method for "tracking" changing parameters.

CHAPTER V

CONCLUSIONS

Since most physical processes are subject to some degree of uncertainty in process parameters, a parameter sensitivity analysis will give an accuracy requirement for the control policy. The parameter sensitivity of optimal and suboptimal control policies of two batch reactions have been presented in Chapters III and IV respectively. It was found that Millman's proportional control policy is less sensitive than the optimal control policy to changes in kinetic parameters. For the complex reaction example, control policy based on an instantaneous performance index is quite sensitive for certain conditions. It was found that the suboptimal control policies result in final yields which are quite close to the optimal control policy when no noise is involved in the measurements and the kinetic parameters are known a priori. Hence suboptimal control policies, as investigated in this thesis, seem to be a practical approach.

For the batch reaction examples investigated in this thesis, the proposed nonlinear filter algorithms provide a feasible approach for tracking unknown parameters. Even for large sampling time intervals, high measurement noise levels and inaccurate initial states, the filter algorithms resulted in encouraging parameter estimations. When the computation time and computer storage are critical factors, the simplified filter algorithms provide a reasonable approach.

A filter included in the feedback control loop can track

uncertain or changing parameters and improve the final yields of the desired products.

Since the suboptimal control policies require knowledge of the current state of the process, the control policies cannot be implemented when some of the required state variables are inaccessible. However, a nonlinear filter in the control loop can also provide the required state estimates from the measurement data and thus overcome this shortcoming of many suboptimal control policies.

NOTATION

Symbol	Description
A_i	i -th chemical species
c	extent of reaction
C_i, C_{i0}	concentration of A_i
C_p	total heat capacity per unit volume
E_i	activation energy
$\hat{E}_i$	estimated E_i
$E_{i,ref}$	fixed reference value of E_i
$\underline{f}(\underline{x}, t)$	vector function
f_i	i -th component of $\underline{f}(\underline{x}, t)$
f_{ij}	$\partial f_i(\underline{x}, t) / \partial x_j$
$\underline{g}(\underline{z}, \underline{p}, t)$	vector function
$\underline{h}(\underline{x}, t)$	vector function
(ΔH)	heat of reaction (negative for exothermic reaction)
J	$(-\Delta H) / C_p$
k_i'	frequency factor
$\underline{\underline{K}}(\underline{x}, t)$	matrix function
K_1, K_2	proportional controller constant
ℓ	dimension of unknown input vector
m	dimension of measurement vector
n	dimension of state vector (including unknown parameter)
$\underline{p}$	parameter vector
$\underline{\underline{P}}(t)$	covariance matrix of state vector $\underline{x}(t)$
P_{ij}	element of $\underline{\underline{P}}(t)$
q'	rate of heat removal

q'_m	optimal value of q'
q	q'/C_p
q_m	optimal value of q
$\underline{\underline{Q}}(t)$	weighting matrix
$r(c,T), r_i$	reaction rates
$r_m(c,T)$	optimal value of $r(c,T)$
R	gas constant
t	time
t_b	total batch processing time
t_f	fixed final time
t_p	update interval of $\underline{\underline{P}}(t)$
t_s	data sampling interval
T	temperature
$\hat{T}$	estimated temperature
T_m	optimal value of T
$\underline{v}(t)$	measurement noise vector
$\underline{\underline{V}}(\underline{x}, t)$	matrix function
$\underline{w}(t)$	unknown input vector
$\underline{\underline{W}}(t)$	weighting matrix
$\underline{x}(t)$	argumented state vector (including parameters)
$x_i(t)$	i -th component of $\underline{x}(t)$
$\hat{\underline{x}}(t)$	estimate of $\underline{x}(t)$
$\hat{x}_i(t)$	i -th component of $\hat{\underline{x}}(t)$
$\underline{y}(t)$	measurement vector
$\underline{z}(t)$	state vector

α_i	stoichiometric coefficient
β_i	forward reaction order
γ_i	backward reaction order
ξ_i	$\beta_i - \gamma_i$
ρ	$E_1/(E_2 - E_1)$
σ	standard deviation
$\varepsilon(0, \sigma), \varepsilon_i(0, \sigma)$	Gaussian distributed random noise with zero mean and standard deviation σ

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APPENDIX A

DERIVATION OF DETCHMENDY AND SRIDHAR NONLINEAR FILTER [22,31]

In this appendix, Detchmندی and Sridhar nonlinear filter [22] based on the derivation presented by Sage [31] is derived. First, the Pontryagin maximum principle corresponding to the Bolza problem in the calculus of variations is discussed. Then the optimal estimation problem using a weighted least squares criterion is formulated. Finally the invariant imbedding technique is employed to solve the resulting two point boundary value problem. After certain approximations are made, the final filter equations are resulted.

The Bolza Problem In The Calculus Of Variations

Consider a given nonlinear system operating over the fixed time interval $t_0 \leq t \leq t_f$ of the form

$$\dot{\underline{x}} = \underline{f}(\underline{x}, \underline{u}, t) \quad (A-1)$$

where $\underline{x}(t)$, the n-vector of state variables, is determined by $\underline{u}(t)$, the m-vector of control variables.

It is desired to determine the control vector $\underline{u}(t)$ such that the following cost function is minimized

$$I = \theta[\underline{x}(t), t] \Big|_{t=t_0}^{t=t_f} + \int_{t_0}^{t_f} \phi[\underline{x}(t), \underline{u}(t), t] dt \quad (A-2)$$

Next, the Lagrange multiplier $\underline{\lambda}$ is used to adjoin the system differential equality constraint (i.e. Equation (A-1)) to the cost function, which gives

$$I = \theta[\underline{x},(t),t] \Big|_{t=t_0}^{t=t_f} + \int_{t_0}^{t_f} \{ \phi[\underline{x}(t),\underline{u}(t),t] + \underline{\lambda}' [\underline{f}(\underline{x},t) - \dot{\underline{x}}] \} dt \quad (A-3)$$

where $\underline{\lambda}'$ is the transpose of $\underline{\lambda}$.

Define a scalar Hamiltonian function as

$$H[\underline{x},\underline{u},\underline{\lambda},t] = \phi[\underline{x}(t),\underline{u}(t),t] + \underline{\lambda}' [\underline{f}(\underline{x},\underline{u},t) - \dot{\underline{x}}] \quad (A-4)$$

Then the cost function becomes

$$I = \theta[\underline{x},t] \Big|_{t=t_0}^{t=t_f} + \int_{t_0}^{t_f} \{ H[\underline{x},\underline{u},\underline{\lambda},t] - \underline{\lambda}' \dot{\underline{x}} \} dt \quad (A-5)$$

Integrating the last term in the integrand of Equation (A-5) by parts, gives

$$I = \{ \theta[\underline{x},t] - \underline{\lambda}' \underline{x} \} \Big|_{t=t_0}^{t=t_f} + \int_{t_0}^{t_f} \{ H[\underline{x},\underline{u},\underline{\lambda},t] + \dot{\underline{\lambda}}' \underline{x} \} dt \quad (A-6)$$

For small variations in the control vectors (and consequently the state vectors) from their optimal values, the resulting deviation in I is given by

$$\begin{aligned} \Delta I &= I[\underline{x} + \delta \underline{x}, \dot{\underline{x}} + \delta \dot{\underline{x}}, \underline{u} + \delta \underline{u}] - I[\underline{x}, \dot{\underline{x}}, \underline{u}] \\ &= \{ \theta[\underline{x} + \delta \underline{x}, t] - \underline{\lambda}' (\underline{x} + \delta \underline{x}) \} \Big|_{t=t_0}^{t=t_f} + \int_{t_0}^{t_f} \{ H[\underline{x} + \delta \underline{x}, \dot{\underline{x}} + \delta \dot{\underline{x}}, \\ &\quad \underline{u} + \delta \underline{u}, t] + \dot{\underline{\lambda}}' (\underline{x} + \delta \underline{x}) \} dt - \{ \theta[\underline{x}, t] - \underline{\lambda}' \underline{x} \} \Big|_{t=t_0}^{t=t_f} \\ &\quad - \int_{t_0}^{t_f} \{ H[\underline{x}, \dot{\underline{x}}, \underline{u}, t] + \dot{\underline{\lambda}}' \underline{x} \} dt \end{aligned} \quad (A-7)$$

A Taylor series expansion is then made and truncated after the first order terms(i.e. $\delta \underline{x}$, $\delta \underline{u}$). The resulting change in I is referred to as the first variation of I , denoted by δI , and is given by

$$\delta I = \left\{ \delta \underline{x}' \left[\frac{\partial \theta}{\partial \underline{x}} - \underline{\lambda} \right] \right\} \Big|_{t=t_0}^{t=t_f} + \int_{t_0}^{t_f} \left\{ \delta \underline{x}' \left[\frac{\partial H}{\partial \underline{x}} + \dot{\underline{\lambda}} \right] + \delta \underline{u}' \left[\frac{\partial H}{\partial \underline{u}} \right] \right\} dt \quad (A-8)$$

A necessary condition for an extremum of I is that δI vanish for arbitrary $\delta \underline{x}$ and $\delta \underline{u}$. Thus it is obtained

$$\dot{\underline{\lambda}} = - \frac{\partial H}{\partial \underline{x}} \quad (A-9)$$

$$\dot{\underline{x}} = \underline{f}(\underline{x}, \underline{u}, t) = \frac{\partial H}{\partial \underline{\lambda}} \quad (A-10)$$

$$\frac{\partial H}{\partial \underline{u}} = \underline{0} \quad (A-11)$$

and the transversality conditions

$$\delta \underline{x}' \left[\frac{\partial \theta}{\partial \underline{x}} - \underline{\lambda} \right] = \underline{0} \quad \text{at } t = t_0, t_f \quad (A-12)$$

Estimation Problem

The Bolza problem in the calculus of variations has just been discussed. Now consider a nonlinear system with the dynamic equation

$$\dot{\underline{x}}(t) = \underline{f}(\underline{x}, t) + \underline{K}(\underline{x}, t) \underline{w}(t) \quad (A-13)$$

and the observation equation

$$\underline{y}(t) = \underline{h}(\underline{x}, t) + \underline{v}(t) \quad (A-14)$$

where

$\underline{x}$ = n-state vector (including unknown parameters)

$\underline{f}(\underline{x},t)$ = n vector function , $\underline{h}(\underline{x},t)$ = m vector function

$\underline{K}(\underline{x},t)$ = n x ℓ matrix , $\underline{y}(t)$ = m vector of outputs

$\underline{w}(t)$ = ℓ vector of unknown inputs , $\underline{v}(t)$ = m vector of measurement errors

and the control vector is included in $\underline{f}(\underline{x},t)$.

It is desired to find the least squares estimate of $\underline{x}(t)$, designated by $\hat{\underline{x}}(t)$, such that the following cost function is minimized.

$$\begin{aligned} I &= \int_0^{t_f} [\|\underline{y} - \underline{h}(\hat{\underline{x}},t)\|_{\underline{Q}(t)}^2 + \|\hat{\underline{x}} - \underline{f}(\hat{\underline{x}},t)\|_{\underline{W}(t)}^2] dt \\ &= \int_0^{t_f} [\|\underline{y} - \underline{h}(\hat{\underline{x}},t)\|_{\underline{Q}(t)}^2 + \|\underline{w}\|_{\underline{V}(\hat{\underline{x}},t)}^2] dt \end{aligned} \quad (A-15)$$

where

$$\underline{V}(\hat{\underline{x}},t) = \underline{K}'(\hat{\underline{x}},t) \underline{W}(t) \underline{K}(\hat{\underline{x}},t) \quad (A-16)$$

and

$\|\cdot\|^2$ is the "Euclidean Norm".

Then for the cost function (A-15) and system Equation. (A-13), the Hamiltonian is

$$H(\underline{\hat{x}}, \underline{\lambda}, t) = \|\underline{y}(t) - \underline{h}(\underline{\hat{x}},t)\|_{\underline{Q}(t)}^2 + \|\underline{w}(t)\|_{\underline{V}(\underline{\hat{x}},t)}^2 + \underline{\lambda}'(t) [\underline{f}(\underline{\hat{x}},t) + \underline{K}(\underline{\hat{x}},t) \underline{w}(t)] \quad (A-17)$$

From the previous discussion, by setting $\frac{\partial H}{\partial \underline{w}} = \underline{0}$, it follows that

$$2\underline{V}(\hat{\underline{x}}, t) \underline{w}(t) + \underline{K}'(\hat{\underline{x}}, t) \underline{\lambda} = \underline{0} \quad (\text{A-18})$$

Assume $\underline{V}$ is not singular, then

$$\underline{w}(t) = -\frac{1}{2} \underline{V}^{-1}(\hat{\underline{x}}, t) \underline{K}'(\hat{\underline{x}}, t) \underline{\lambda} \quad (\text{A-19})$$

Substitute Equation (A-19) into Equation (A-17)

$$H(\hat{\underline{x}}, \underline{\lambda}, t) = \|\underline{y}(t) - h(\hat{\underline{x}}, t)\|_{\underline{Q}(t)}^2 + \underline{\lambda}'(t) \underline{f}(\hat{\underline{x}}, t) - \frac{1}{4} \underline{\lambda}'(t) \underline{K}(\hat{\underline{x}}, t) \underline{V}^{-1}(\hat{\underline{x}}, t)$$

$$\underline{K}'(\hat{\underline{x}}, t) \underline{\lambda}(t) \quad (\text{A-20})$$

Then as discussed before, the necessary conditions to have the cost function in Equation (A-15) obtain a minimum value

$$\dot{\hat{\underline{x}}} = \frac{\partial H(\hat{\underline{x}}, \underline{\lambda}, t)}{\partial \underline{\lambda}} \quad (\text{A-21})$$

$$\dot{\underline{\lambda}} = -\frac{\partial H(\underline{x}, \underline{\lambda}, t)}{\partial \hat{\underline{x}}} \quad (\text{A-22})$$

Since t_f is fixed and $\hat{\underline{x}}(0)$, $\hat{\underline{x}}(t_f)$ are free, so the transversality condition, Equation (A-12), yields

$$\underline{\lambda}(0) = \underline{0} \quad (\text{A-23})$$

$$\underline{\lambda}(t_f) = \underline{0} \quad (\text{A-24})$$

With Equations (A-20) to (A-24), a two-point boundary value problem is formulated. To solve this kind of problem, Detchmندی and Sridhar [22] used the invariant imbedding technique and replaced the boundary conditions in (A-26) and (A-27) by the more general conditions

$$\underline{\lambda}(0) = \underline{0} \quad (\text{A-25})$$

$$\underline{\lambda}(t_f) = \underline{C} \quad (\text{A-26})$$

Let the missing final conditions be given by

$$\hat{\underline{x}}(t_f) = \underline{r}(\underline{C}, t_f) \quad (\text{A-27})$$

with $\underline{C}$ and t_f considered to be independent variables. Then by Taylor's expansion, the left hand side of Equation (A-27) becomes,

$$\hat{\underline{x}}(t_f + \Delta t_f) = \hat{\underline{x}}(t_f) + \underline{f}(\hat{\underline{x}}, t) \Delta t + \Delta_1^2 \quad (\text{A-28})$$

and the right hand side of (A-27) becomes,

$$\underline{r}(\underline{C} + \Delta \underline{C}, t_f + \Delta t_f) = \underline{r}(\underline{C}, t_f) + \frac{\partial \underline{r}}{\partial \underline{C}} \Delta \underline{C} + \frac{\partial \underline{r}}{\partial t_f} \Delta t_f + \Delta_2^2 \quad (\text{A-29})$$

and from Equation (A-26),

$$\Delta \underline{C} = - \frac{\partial \underline{H}}{\partial \underline{C}} \Delta t_f + \Delta_3^2 \quad (\text{A-30})$$

where Δ_1^2 , Δ_2^2 and Δ_3^2 represent higher order terms of Δt_f , Δt_f and $\Delta \underline{C}$, and Δt_f respectively and approach zero by taking limits.

Substituting Equation (A-30) into Equation (A-29), equating the right hand sides of Equation (A-28) and Equation (A-29), and taking

limits gives the following invariant imbedding equation

$$\frac{\partial \underline{r}}{\partial t_f} - \left[\frac{\partial \underline{r}}{\partial \underline{C}} \right] \frac{\partial H(\underline{r}, \underline{C}, t_f)}{\partial \underline{r}} = \frac{\partial H(\underline{r}, \underline{C}, t_f)}{\partial \underline{C}} \quad (A-31)$$

Substituting Equation (A-20) into Equation (A-31) gives

$$\begin{aligned} \frac{\partial \underline{r}}{\partial t_f} - \left[\frac{\partial \underline{r}}{\partial \underline{C}} \right] \{ & -2 \underline{h}'(\underline{r}, t_f) \underline{Q}(t_f) [\underline{y}(t_f) - \underline{h}(\underline{r}, t_f)] + \underline{f}'(\underline{r}, t_f) \underline{C} \\ & - \frac{1}{4} \underline{C}' \frac{\partial}{\partial \underline{r}} [\underline{K}(\underline{r}, t_f) \underline{V}^{-1}(\underline{r}, t_f) \underline{K}'(\underline{r}, t_f)] \underline{C} \} \\ & = \underline{f}(\underline{r}, t_f) - \frac{1}{2} \underline{K}(\underline{r}, t_f) \underline{V}^{-1}(\underline{r}, t_f) \underline{K}'(\underline{r}, t_f) \underline{C} \end{aligned} \quad (A-32)$$

where subscripts represent taking derivatives of respective functions.

Assume an approximate solution of $\underline{r}(\underline{C}, t_f)$ of the form^[22]

$$\underline{r}(\underline{C}, t_f) = \hat{\underline{x}}(t_f) - \underline{P}(t_f) \underline{C} \quad (A-33)$$

where $\underline{P}(t_f)$ is an $n \times n$ matrix.

By substituting (A-33) into (A-32) and expanding the result with Taylor's expansion about $\underline{r}(0, t_f)$, it is obtained

$$\begin{aligned} & - \frac{d\underline{P}(t_f)}{dt_f} \underline{C} + \frac{d\hat{\underline{x}}(t_f)}{dt_f} + \underline{P}(t_f) \{ -2 \underline{h}'(\hat{\underline{x}}, t_f) \underline{Q}(t_f) [\underline{y}(t_f) - \underline{h}(\hat{\underline{x}}, t_f)] \\ & + 2 \left[\frac{\partial}{\partial \hat{\underline{x}}} (\underline{h}'(\hat{\underline{x}}, t_f) \underline{Q}(t_f) (\underline{y}(t_f) - \underline{h}(\hat{\underline{x}}, t_f))) \right]' \underline{P} \underline{C} + \underline{f}'(\hat{\underline{x}}, t_f) \underline{C} - \left[\frac{\partial}{\partial \hat{\underline{x}}} (\underline{f}'(\hat{\underline{x}}, t_f) \underline{C}) \right]' \underline{P} \underline{C} \\ & - \frac{1}{4} \underline{C}' \frac{\partial}{\partial \hat{\underline{x}}} [\underline{K}(\underline{x}, t_f) \underline{V}^{-1}(\hat{\underline{x}}, t_f) \underline{K}'(\underline{x}, t_f)] \underline{C} + \frac{1}{4} \left[\frac{\partial}{\partial \hat{\underline{x}}} (\underline{C}' \frac{\partial}{\partial \hat{\underline{x}}} [\underline{K}(\underline{x}, t_f) \underline{V}^{-1}(\hat{\underline{x}}, t_f) \right. \end{aligned}$$

$$\begin{aligned} \underline{\underline{K}}'(\underline{\hat{x}}, t_f) \underline{\underline{C}}] \underline{\underline{C}}] \underline{\underline{P}} \underline{\underline{C}} \} &= \underline{\underline{f}}(\underline{\hat{x}}, t_f) - \underline{\underline{f}}'_{\underline{\hat{x}}} \underline{\underline{P}} \underline{\underline{C}} - \frac{1}{2} \underline{\underline{K}}(\underline{\hat{x}}, t_f) \underline{\underline{V}}^{-1}(\underline{\hat{x}}, t_f) \\ \underline{\underline{K}}'(\underline{\hat{x}}, t_f) \underline{\underline{C}} + \frac{1}{2} \left[\frac{\partial}{\partial \underline{\hat{x}}} (\underline{\underline{K}}(\underline{\hat{x}}, t_f) \underline{\underline{V}}^{-1}(\underline{\hat{x}}, t_f) \underline{\underline{K}}(\underline{\hat{x}}, t_f) \underline{\underline{C}}) \right] \underline{\underline{P}} \underline{\underline{C}} & \quad (A-34) \end{aligned}$$

Collecting terms of zero order $\underline{\underline{C}}$ and those of order higher than zero yields

$$\frac{d\underline{\hat{x}}(t_f)}{dt} = \underline{\underline{f}}(\underline{\hat{x}}, t_f) + \underline{\underline{P}}(t_f) \{ 2 \underline{\underline{h}}'_{\underline{\hat{x}}}(\underline{\hat{x}}, t_f) \underline{\underline{Q}}(t_f) [\underline{\underline{y}}(t_f) - \underline{\underline{h}}(\underline{\hat{x}}, t_f)] \} \quad (A-35)$$

$$\begin{aligned} - \frac{d\underline{\underline{P}}(t_f)}{dt_f} \underline{\underline{C}} &= \{ -\underline{\underline{P}}(t_f) \underline{\underline{f}}'_{\underline{\hat{x}}} - \underline{\underline{f}}'_{\underline{\hat{x}}} \underline{\underline{P}}(t_f) - 2 \underline{\underline{P}}(t_f) \frac{\partial}{\partial \underline{\hat{x}}} [\underline{\underline{h}}'_{\underline{\hat{x}}}(\underline{\hat{x}}, t_f) \underline{\underline{Q}}(t_f) \\ &\quad (\underline{\underline{y}}(t_f) - \underline{\underline{h}}(\underline{\hat{x}}, t_f))] \underline{\underline{P}}(t_f) - \frac{1}{2} \underline{\underline{K}}(\underline{\hat{x}}, t_f) \underline{\underline{V}}^{-1}(\underline{\hat{x}}, t_f) \underline{\underline{K}}(\underline{\hat{x}}, t_f) \\ &\quad + (\text{terms containing } \underline{\underline{C}}' \text{ or } \underline{\underline{C}}) \} \underline{\underline{C}} \quad (A-36) \end{aligned}$$

From Equation (A-36), the terms in the bracket of the right hand side should be equal to $-d\underline{\underline{P}}(t_f)/dt_f$. Since only $\underline{\underline{C}} = \underline{\underline{0}}$ is of interest, the filter equations are obtained as

$$\frac{d\underline{\hat{x}}(t)}{dt} = \underline{\underline{f}}(\underline{\hat{x}}, t) + \underline{\underline{P}}(t) \{ 2 \underline{\underline{h}}'_{\underline{\hat{x}}}(\underline{\hat{x}}, t) \underline{\underline{Q}}(t) [\underline{\underline{y}}(t) - \underline{\underline{h}}(\underline{\hat{x}}, t)] \} \quad (A-37)$$

$$\begin{aligned} \frac{d\underline{\underline{P}}(t)}{dt} &= \underline{\underline{P}}(t) \underline{\underline{f}}'_{\underline{\hat{x}}}(\underline{\hat{x}}, t) + \underline{\underline{f}}'_{\underline{\hat{x}}}(\underline{\hat{x}}, t) \underline{\underline{P}}(t) + 2 \underline{\underline{P}}(t) \left\{ \frac{\partial}{\partial \underline{\hat{x}}} [\underline{\underline{h}}'_{\underline{\hat{x}}}(\underline{\hat{x}}, t) \right. \\ &\quad \left. \underline{\underline{Q}}(t) (\underline{\underline{y}}(t) - \underline{\underline{h}}(\underline{\hat{x}}, t))] \right\} + \frac{1}{2} \underline{\underline{K}}(\underline{\hat{x}}, t) \underline{\underline{V}}^{-1}(\underline{\hat{x}}, t) \underline{\underline{K}}'(\underline{\hat{x}}, t) \quad (A-38) \end{aligned}$$

APPENDIX B

In this appendix two computer programs are listed. One is the program written to estimate the unknown parameter E_1 of the single reaction example in Chapter III. The other program estimates the unknown parameters E_4 and E_5 of the complex reaction example in Chapter IV. Both of the programs are written for the Filter I algorithm. Modifications of the program can be made to investigate the effects of noise level and data sampling interval on filter estimation. A change of one program statement in the listed program results in the Filter II algorithm. For Filter III algorithm, a change in a function evaluates subroutine becomes necessary as is indicated in the appropriate place in the program.

C MAINLINE SMPX

C MAINLINE SMPX

```

C      *****
C      *
C      *                      MAINLINE        SMPX                      *
C      *                      -----                                      *
C      *
C      *      PURPOSE                                                              *
C      *              THIS PROGRAM IS WRITTEN BY USING DETCHMENDY              *
C      *              AND SRIDHAR NONLINEAR FILTER TO IDENTIFY THE              *
C      *              UNKNOWN ACTIVATION ENERGY OF A SINGLE RE-              *
C      *              ACTION EXAMPLE(CHIEN AND ARIS)                              *
C      *
C      *      PARAMETER DESCRIPTIONS                                              *
C      *              Y(1).....EXTENT OF REACTION                              *
C      *              Y(2).....STATE VARIABLE CORRESPONDING                      *
C      *                                      TO TEMPERATURE                      *
C      *              Y(3).....STATE VARIABLE CORRESPONDING                      *
C      *                                      TO UNKNOWN E1                      *
C      *              PRMT(1).....LOWERBOUND OF TIME                              *
C      *              PRMT(3).....SAMPLING INTERVAL                              *
C      *              PRMT(2).....UPPERBOUND OF TIME                              *
C      *              NDIM.....DIMENSION OF STATE VARIABLE                      *
C      *              HR.....FORWARD FREQ. FACTOR                              *
C      *              HB.....BACKWARD FREQ. FACTOR                              *
C      *              Q(I,J).....COVARIANCE DIFFERENTIAL MATRIX                      *
C      *                                      OF NONLINEAR FILTER                      *
C      *              CT.....THE ESTIMATE OF TEMPERATURE                              *
C      *              EA.....THE ESTIMATE OF ACTIVATION                              *
C      *                                      ENERGY OF E1                              *
C      *              TM.....THE MEASURED TEMPERATURE                              *
C      *
C      *      SUBROUTINE CALLED AND USAGE                                              *
C      *              CALL RKGMM                                                      *
C      *              I.E. RUNGE-KUTTA-GILL INTEGRATION ROUTINE                      *
C      *
C      *              CALL GAUSS(IX,S,AM,V)                                              *
C      *              I.E. GAUSSIAN RANDOM NUMBER GENERATOR                              *
C      *              (IBM 360 SSP ROUTINE)                                              *
C      *                                                                              S
C      *
C      *              WHERE                                                              *
C      *                      IX IS AN ARBITRARY INTEGER(POSITIVE)                      *
C      *                      S IS THE STANDARD DEVIATION                              *
C      *                      AM IS THE ARITHMETIC MEAN                              *
C      *                      V IS THE GENERATED RANDOM NUMBER                              *
C      *                                                                              *
C      *      *****

```

INTEGER PA
 DIMENSION RRX(1700),RCA(1700),RTP(1700)

C MAINLINE SMPX ... (CONT'D)

```
COMMON PRMT(3),X,NDIM,Y(12),DERY(12)
COMMON R,HR,HB,Q(3,3),CJ,CX,ZH(3),CCX,TM,QINT
```

C SPECIFY THE VALUES OF PRMT(1),PRMT(2),PRMT(3)

```
PRMT(1)=0.
PRMT(2)=1700.
PRMT(3)=1.
X=PRMT(1)
```

C SPECIFY THE INITIAL STATE VARIABLES

```
Y(1)=0.
Y(2)=0.
Y(3)=0.1
WRITE(6,11)
11 FORMAT('0',15X,'NONLINEAR FILTER ESTIAMTION OF STATES
* AND UNKNOWN
*PARAMETER')
WRITE(6,22)
22 FORMAT('///',3X,'*PROCESS',17X,'SET*',4X,'*ESTIMATION'
*,27X,'SET*','/'0
*,5X,'TIME',5X,'CONC.',7X,'TEMP.',6X,'TIME',6X,'CONC.'
*,7X,'TEMP.',
*9X,'Q(1,1)',5X,'Q(2,2)',4X,'Q(3,3)'/)
R=2.
HR=EXP(12.)
HB=EXP(30.)
CJ=400./100.
```

C SPECIFY THE INITIAL COVARIANCE DIFFERENTIAL MATRIX

```
DO 9 I=1,3
DO 9 J=1,3
Q(I,J)=0.
9 CONTINUE
Q(1,1)=0.0025
Q(2,2)=0.01
Q(3,3)=1.
```

C CHANGE THE Q(I,J) MATRIX TO STATE VARIABLES OF FILTER

C MAINLINE SMPX ... (CONT'D)

```

K=0
DO 10 I=1,3
K=K+2
DO 10 J=1,3
IJK=I+J+K
Y(IJK)=Q(I,J)
10 CONTINUE

```

C SPECIFY THE PARAMETER VALUES OF SUBROUTINE GAUSS

```

IX=1111
S=1.
AM=0.

PA=PRMT(2)/PRMT(3)
N=PA
X=PRMT(1)
ZH(1)=0.
ZH(2)=0.
ZH(3)=0.
EX=5.
CX=5.

```

C READ IN ALL THE PROCESS DATA

```

IJ=1
40 KJ=IJ+4
READ(5,33)(RRX(I),RCA(I),RTP(I),I=IJ,KJ)
33 FORMAT(5(3A4))
IJ=KJ+1
IF(KJ.EQ.1700)GO TO 70
GO TO 40
70 INT=PRMT(3)
MN=0

```

C READ IN THE UPDATE INTERVAL(IQIN)FOR THE FILTER 2
C ALGORITHM

C IF IQIN=PRMT(3) MEANS FILTER 1 ALGORITHM

```

READ(5,71)IQIN
71 FORMAT(I4)

```


C MAINLINE SMPX ... (CONT'D)

```
      ISET=IQIN
60  MN=MN+INT
      XA=RRX(MN)
      CA=RCA(MN)
      TP=RTP(MN)
      CALL GAUSS(IX,S,AM,V)
      TM=TP+V
      IF(MN.EQ.IQIN)NDIM=12
      IF(NDIM.EQ.12)IQIN=IQIN+ISET
      IF(NDIM.EQ.12)GO TO 65
      NDIM=3
65  CONTINUE
      CALL RKGM
      IF(X.LT.EX)GO TO 60
      EX=EX+5.
      CT=500.+100.*Y(2)
      EA=(1.+Y(3))*24000.
      WRITE(6,43)XA,CA,TP,X,Y(1),CT,EA,Y(4),Y(8),Y(12)
43  FORMAT(' ',3X,F7.2,3X,F8.4,3X,F9.3,3X,F7.2,3X,F8.4,3X
*,F9.3,3X,E13.
*,5,3(2X,E10.3))
      IF(X.GE.PRMT(2))GO TO 100
      IF(CT.LT.300)GO TO 100
      GO TO 60
100 STOP
      END
```


C SUBROUTINE FCT

C SUBROUTINE FCT

```

C *****
C *
C * SUBROUTINE FCT
C * -----
C *
C * PURPOSE
C * THIS SUBROUTINE INCLUDE THE NONLINEAR FILTER
C * EQUATIONS AND SUPPLY THE NUMERICAL DATA
C * TO SUBROUTINE RKGM FOR INTEGRATION
C *
C *****

```

SUBROUTINE FCT

```

DIMENSION FX(3),DFX(3,3),FQ(3,3),QF(3,3),ZC(3,3),QZ(3
*,3),QZQ(3,3)
DIMENSION EQ(3,3),EY(12),QH(3),EFX(2)
COMMON PRMT(3),X,NDIM,Y(12),DERY(12)
COMMON R,HR,HB,Q(3,3)
COMMON CJ,CX,ZH(3),CCX,TM
CR=(3.-Y(1))*(2.-Y(1))
CB=(1.+Y(1))*2
CFR=-5.+2.*Y(1)
CFB=2.*(1.+Y(1))
EP=24000.
CT=500.+100.*Y(2)
EA=(1.+Y(3))*EP
ACR=EXP((-EA/CT)/R)
BE=EA+24000.
ACB=EXP((-BE/CT)/R)
FX(1)=HR*ACR*CR-HB*ACB*CB
FX(2)=CJ*FX(1)
FX(3)=0.
TE=500.+100.*Y(2)
ZH(2)=(TM-TE)/100.
IF(NDIM.EQ.12)GO TO 110

```

C IF NDIM=12 MEANS FILTER 1 ALGORITHM

C FILTER 3 ALGORITHM FOR EVALUATION OF Q(I,J) IS PUT IN
C HERE

```

DO 120 I=1,3
120 QH(I)=0.
DO 125 I=1,3

```


C SUBROUTINE FCT ... (CONT'D)

```

DO 125 J=1,3
125 QH(I)=QH(I)+Q(I,J)*ZH(J)
DO 130 I=1,3
130 DERY(I)=FX(I)+QH(I)
GO TO 99
110 RT2=R*CT**2
EER=EA/RT2
EEB=BE/RT2
RT1=-R*CT

```

C FOR FILTER 3 ALGORITHM THE FOLLOWING IS DELETED

C CALCULATE THE JACOBIAN

```

DFX(1,1)=HR*ACR*CFR-HB*ACB*CFB
DFX(1,2)=(HR*ACR*CR*EER-HB*ACB*EEB*CB)*100.
DFX(1,3)=((HR*ACR*CR)/RT1-(HB*ACB*CB)/RT1)*(24000.)
DFX(2,1)=CJ*DFX(1,1)
DFX(2,2)=CJ*DFX(1,2)
DFX(2,3)=CJ*DFX(1,3)
DFX(3,1)=0.
DFX(3,2)=0.
DFX(3,3)=0.
K=0
DO 100 I=1,3
K=K+2
DO 100 J=1,3
IJK=I+J+K
Q(I,J)=Y(IJK)
100 CONTINUE
DO 10 I=1,3
DO 10 J=1,3
FQ(I,J)=0.
GF(I,J)=0.
10 CONTINUE
DO 20 K=1,3
DO 20 I=1,3
DO 20 J=1,3
FQ(K,I)=FQ(K,I)+DFX(K,J)*Q(J,I)
20 CONTINUE
DO 30 K=1,3
DO 30 I=1,3
DO 30 J=1,3
QF(K,I)=QF(K,I)+Q(K,J)*DFX(I,J)
30 CONTINUE
DO 40 I=1,3

```


C SUBROUTINE FCT ... (CONT'D)

```
QH(I)=0.
DO 40 J=1,3
  ZC(I,J)=0.
  QZ(I,J)=0.
  QZQ(I,J)=0.
40 CONTINUE
  ZC(2,2)=1.
  DO 50 K=1,3
    DO 50 I=1,3
      DO 50 J=1,3
        QZ(K,I)=QZ(K,I)+Q(K,J)*ZC(J,I)
50 CONTINUE
    DO 60 K=1,3
      DO 60 I=1,3
        DO 60 J=1,3
          QZQ(K,I)=QZQ(K,I)+QZ(K,J)*Q(J,I)
60 CONTINUE
    DO 70 I=1,3
      DO 70 J=1,3
        EQ(I,J)=FQ(I,J)+QF(I,J)-QZQ(I,J)
70 CONTINUE
    K=0
    DO 80 I=1,3
      K=K+2
      DO 80 J=1,3
        KIJ=K+I+J
        EY(KIJ)=EQ(I,J)
80 CONTINUE
    DO 95 I=1,3
      DO 95 J=1,3
        QH(I)=QH(I)+Q(I,J)*ZH(J)
95 CONTINUE
    DO 85 I=1,3
      EY(I)=FX(I)+QH(I)
85 CONTINUE
    DO 90 I=1,12
      DERY(I)=EY(I)
90 CONTINUE
99 RETURN
END
```


C SUBROUTINE RKGM

C SUBROUTINE RKGM

```

C *****
C *
C * SUBROUTINE RKGM
C * -----
C *
C * FUNCTION OF THIS SUBROUTINE
C *
C * RUNGE-KUTTA-GILL INTEGRATION ROUTINE
C *
C * PARAMETER DESCRIPTIONS
C * X.....THE INDEPENDENT VARIABLE
C * NDIM.....DIMENSION OF DEPENDENT VARI-
C * ABLES
C * Y(I).....THE DEPENDENT VARIABLES WITH
C * DIMENSION NDIM
C * PRMT(3).....INTEGRATION INTERVAL
C * DERY(I).....DERIATIVE OF STATE FUNCTIONS
C *
C * SUBROUTINE CALLED AND USAGE
C *
C * CALL FCT
C *
C *****

```

SUBROUTINE RKGM

```

DIMENSION RJ(27),RK(27),RQ(27)
COMMON PRMT(3),X,NDIM,Y(12),DERY(12)
COMMON R,HR,HB,Q(3,3),CJ,CX,ZH(3),CCX,TM,QINT
H=PRMT(3)
5 RX=X
DO 10 I=1,NDIM
10 RJ(I)=Y(I)
CALL FCT
DO 20 I=1,NDIM
20 RK(I)=H*DERY(I)
DO 30 I=1,NDIM
RJ(I)=RJ(I)+0.5*RK(I)
30 RQ(I)=RK(I)
X=RX+H/2.
DO 40 I=1,NDIM
40 Y(I)=RJ(I)
CALL FCT
DO 50 I=1,NDIM
50 RK(I)=H*DERY(I)
SQ=1./SQRT(2.)

```


C SUBROUTINE RKGM ... (CONT'D)

```
60 RJ(I)=RJ(I)+(1.-SQ)*(RK(I)-RQ(I))
   CA=2.-SQRT(2.)
   CB=-2.+3./SQRT(2.)
   DO 70 I=1,NDIM
70 RQ(I)=CA*RK(I)+CB*RQ(I)
   DO 80 I=1,NDIM
80 Y(I)=RJ(I)
   CALL FCT
   DO 90 I=1,NDIM
   RK(I)=H*DERY(I)
90 RJ(I)=RJ(I)+(1.+SQ)*(RK(I)-RQ(I))
   CE=2.+SQRT(2.)
   CF=-2.-3./SQRT(2.)
   DO 100 I=1,NDIM
100 RQ(I)=CE*RK(I)+CF*RQ(I)
   X=RX+H
   DO 110 I=1,NDIM
110 Y(I)=RJ(I)
   CALL FCT
   DO 120 I=1,NDIM
120 RK(I)=H*DERY(I)
   DO 130 I=1,NDIM
130 Y(I)=RJ(I)+RK(I)/6.-RQ(I)/3.
   CALL FCT
6 RETURN
END
```


C MAINLINE CMPX

C MAINLINE CMPX

[illegible]

C MAINLINE CMPX ... (CONT'D)

```

C      ****
      DIMENSION PY(3),QY(3)
      COMMON X,Y(27),DERY(27),PRMT(3),FREQ(5),EK(5),Q(6,6)
      *,WF(3,3),HD(3,
      *6),THD(6,3),ZH(3),NDIM,ACTIVE(5),ACTV2,ACTV4,ACTV5,L
      *,TEMP
      COMMON RCONC(3)
      READ(5,5)(ACTIVE(I),I=1,5)
5    FORMAT(5F5.0)
      READ(5,10)(FREQ(I),I=1,5)
10   FORMAT(5F5.4)
      WRITE(6,15)
15   FORMAT('0',10X,'ON-LINE IDENTIFICATION OF KINETIC
      * PARAMETERS')
      WRITE(6,20)
20   FORMAT('0',15X,'ACTUAL ACTIVATION ENERGY AS
      * FOLLOWING')
      WRITE(6,25)(ACTIVE(I),I=1,5)
25   FORMAT('0',10X,'E1=',F5.0,3X,'E2=',F5.0,3X,'E3=',F5.0
      *,3X,'E4=',F5.
      *0,3X,'E5=',F5.0)
      COFF1=0.8
      COFF2=1.2
      ACTIVE(4)=COFF1*ACTIVE(4)
      ACTIVE(5)=COFF2*ACTIVE(5)
      ACTV4=ACTIVE(4)
      ACTV5=ACTIVE(5)

C      ACTV4,ACTV5 ARE THE THE INITIAL GUESSED E4 AND E5

      WRITE(6,30)
30   FORMAT('0',15X,'MODEL ACTIVATION ENERGY AS FOLLOWING')
      WRITE(6,35)(ACTIVE(I),I=1,3),ACTV4,ACTV5
35   FORMAT('0',10X,'E1=',F6.1,3X,'E2=',F6.1,3X,'E3=',F6.1
      *,3X,'E4=',F6.
      *1,3X,'E5=',F6.1)
      WRITE(6,38)
38   FORMAT('0',25X,'ESTIMATION',16X,'SET',35X,'PROCESS',7X
      *,'SET')
      WRITE(6,40)
40   FORMAT('0',5X,'TIME',4X,'C(A)',4X,'C(C)',4X,'C(D)',9X
      *,',K2',13X,'K4
      *,',14X,'K5',8X,'TIME',3X,'C(A)',3X,'C(C)',3X,'C(D)')

C      SPECIFY THE VALUES OF PRMT(1)

      PRMT(2)=1.
      PRMT(1)=0.
      PRMT(3)=0.005

```


C MAINLINE CMPX ... (CONT'D)

X=PRMT(1)

C SPECIFY THE INITIAL ESTIMATS OF STATES

Y(1)=1.
Y(2)=0.
Y(3)=0.
Y(4)=0.
Y(5)=0.

C SPECIFY THE VALUES OF COVARIANCE MATRIX Q(I,J)

DO 60 I=1,5
DO 60 J=1,5
Q(I,J)=0.5
60 CONTINUE
Q(4,4)=250.
Q(5,5)=250.
DO 61 I=1,3
DO 61 J=1,5
HD(I,J)=0.
61 CONTINUE
HD(1,1)=1.
HD(2,2)=1.
HD(3,3)=1.
DO 62 I=1,3
DO 62 J=1,5
THD(J,I)=HD(I,J)
62 CONTINUE

C CHANGE THE COVARIENCE MATRIC Q(I,J) INTO STATE
C VARIABLES OF FILTER EQUATIONS

K=0
DO 65 I=1,5
K=K-I+5
DO 65 J=I,5
IJK=I+J+K
Y(IJK)=Q(I,J)
65 CONTINUE

C WEIGHTING FACTOR

DO 70 I=1,3
DO 70 J=1,3
WF(I,J)=0.
70 CONTINUE
WF(1,1)=1.
WF(2,2)=1.
WF(3,3)=1.

C MAINLINE CMPX ... (CONT'D)

```

DO 75 I=1,3
ZH(I)=0.
75 CONTINUE
TEMP=1120.
IX=9
SD=0.1
AM=0.

```

C SPECIFY THE UPDATE INTERVAL(IQIN) OF FILTER 2
C ALGORITHM
C IF IQIN=1 MEAS FILTER 1 ALGORITHM

```

IQIN=1
ISET=IQIN
ITIME=0
PX=X
DO 76 I=1,3
PY(I)=Y(I)
76 CONTINUE
74 CONTINUE
ITIME=ITIME+1

```

C L=1 I.E. SECTION TO GERENATE PROCESS DATA

```

L=1
NDIM=3
CALL RKGM
QX=X
DO 77 I=1,3
QY(I)=Y(I)
77 CONTINUE
X=PX
DO 78 I=1,3
Y(I)=PY(I)
78 CONTINUE
DO 79 I=1,3
CALL GAUSS(IX,SD,AM,RDN)
RCONC(I)=QY(I)*(1.+RDN)
IF(ITIME.LT.IQIN)NDIM=5
IF(ITIME.EQ.IQIN)NDIM=20
IF(ITIME.EQ.IQIN)IQIN=IQIN+ISET

```

C L=2 I.E. FILTERING SECTION

```

L=2
79 CONTINUE
CALL RKGM

```

C IPI FEEDBACK CONTROL POLICY

C MAINLINE CMPX ... (CONT'D)

```
TEMP1=TEMP
YB=1.-Y(1)-Y(2)-Y(3)
YC=Y(2)
A=FREQ(4)*ACTIVE(4)*YB
B=FREQ(5)*ACTIVE(5)*YC
AB=A/B
IF(AB.LT.0.)GO TO 31
IF(IDEN.EQ.2)GO TO 22
IF(X.EQ.0.)GO TO 12
PA=(ACTIVE(4)-ACTIVE(5))/ALOG(AB)
PB=1./PA+1./658.
TEMP=1./PB
IF(TEMP.GE.1120.)GO TO 12
IF(TEMP.LT.0.)GO TO 12
IDEN=2
GO TO 32
12 CONTINUE
TEMP=1120.
GO TO 32
22 CONTINUE
PA=(ACTIVE(4)-ACTIVE(5))/ALOG(AB)
PB=1./PA+1./658.
TEMP=1./PB
IF(TEMP.LT.850.)TEMP=850.
GO TO 32
31 CONTINUE
TEMP=TEMP1
32 CONTINUE
IF(TEMP.GT.TEMP1)TEMP=TEMP1
IF(TEMP.LT.850.)TEMP=850.
PX=X
DO 80 I=1,3
PY(I)=Y(I)
80 CONTINUE
X=QX
DO 81 I=1,3
Y(I)=QY(I)
81 CONTINUE
IF(X.LT.PRMT(2))GO TO 74
100 STOP
END
```


C SUBROUTINE FCT

C SUBROUTINE FCT

```

C      ****
C      *
C      *               SUBROUTINE FCT
C      *               -----
C      *
C      *   PURPOSE
C      *       THIS SUBROUTINE INCLUDE THE NONLINEAR FILTER
C      *       EQUATIONS AND SUPPLY THE REQUIRED NUMERICAL
C      *       DATA FOR SUBROUTINE RKGM FOR INTEGRATION
C      *
C      ****

```

```

SUBROUTINE FCT
  DIMENSION WZ(3),QH(6,3),QW(6),EY(27),FX(6),DFX(6,6)
  *,FQ(6,6),QF(6,6)
  *,QWH(6,6),QWQ(6,6),EQ(6,6),WH(3,6)
  COMMON X,Y(27),DERY(27),PRMT(3),FREQ(5),EK(5),Q(6,6)
  *,WF(3,3),HD(3,
  *,6),THD(6,3),ZH(3),NDIM,ACTIVE(5),ACTV2,ACTV4,ACTV5,L
  *,TEMP
  COMMON RCONC(3)
  CONST=1./TEMP-1./658.
  EK(1)=FREQ(1)*EXP(-8000.*CONST)
  EK(2)=FREQ(2)*EXP(-7000.*CONST)
  EK(3)=FREQ(3)*EXP(-7500.*CONST)
  GO TO (1,3),L
1 CONTINUE
  EK(4)=FREQ(4)*EXP(-5000.*CONST)
  EK(5)=FREQ(5)*EXP(-7500.*CONST)
  FX(1)=-(EK(1)+EK(2)+EK(3))*Y(1)
  FX(2)=(1.-(Y(1)+Y(2)+Y(3)))*EK(4)-EK(5)*Y(2)
  FX(3)=(EK(2)+EK(3))*Y(1)+EK(5)*Y(2)
  DO 2 I=1,3
    DERY(I)=FX(I)
2 CONTINUE
  GO TO 141
3 CONTINUE
  ACTIVE(4)=ACTV4*Y(4)+ACTV4
  ACTIVE(5)=ACTV5*Y(5)+ACTV5
  EK(4)=FREQ(4)*EXP(-ACTIVE(4)*CONST)
  EK(5)=FREQ(5)*EXP(-ACTIVE(5)*CONST)
  FX(1)=-(EK(1)+EK(2)+EK(3))*Y(1)
  FX(2)=(1.-(Y(1)+Y(2)+Y(3)))*EK(4)-EK(5)*Y(2)
  FX(3)=(EK(2)+EK(3))*Y(1)+EK(5)*Y(2)
  FX(4)=0.
  FX(5)=0.
  ZH(1)=RCONC(1)-Y(1)
  ZH(2)=RCONC(2)-Y(2)

```


C SUBROUTINE FCT ... (CONT'D)

ZH(3)=RCONC(3)-Y(3)

C CALCULATION OF Q(I,J) ARE PUT IN HERE FOR FILTER 3

K=0

DO 20 I=1,5

K=K-I+5

IJ=I

DO 20 J=IJ,5

IJK=I+J+K

Q(I,J)=Y(IJK)

20 CONTINUE

DO 30 I=1,5

IJ=I

DO 30 J=IJ,5

Q(J,I)=Q(I,J)

30 CONTINUE

DO 40 J=1,3

WZ(J)=0.

DO 40 I=1,5

QW(I)=0.

QH(I,J)=0.

40 CONTINUE

DO 45 K=1,5

DO 45 I=1,3

DO 45 J=1,5

QH(K,I)=QH(K,I)+Q(K,J)*THD(J,I)

45 CONTINUE

DO 50 I=1,3

DO 50 J=1,3

WZ(I)=WZ(I)+WF(I,J)*ZH(J)

50 CONTINUE

DO 55 I=1,5

DO 55 J=1,3

QW(I)=QW(I)+QH(I,J)*WZ(J)

55 CONTINUE

C ESTIMATION EQUATION OF STATE VARIABLE INCLUDING
C UNKNOWN
C PARAMETERS

DO 60 I=1,5

EY(I)=FX(I)+QW(I)

60 CONTINUE

IF(NDIM.EQ.20)GO TO 62

DO 61 I=1,NDIM

DERY(I)=EY(I)

61 CONTINUE

IF(NDIM.EQ.5)GO TO 141

62 CONTINUE

C SUBROUTINE FCT ... (CONT'D)

C WHEN FILTER 3 ALGORITHM IS USED THE FOLLOWING IS
C DELETED

```

DO 10 I=1,5
DO 10 J=1,5
DFX(I,J)=0.
10 CONTINUE
DFX(1,1)=-(EK(1)+EK(2)+EK(3))
DFX(2,1)=-EK(4)
DFX(2,2)=-EK(4)-EK(5)
DFX(2,3)=-EK(4)
DFX(2,4)=(1.-(Y(1)+Y(2)+Y(3)))*EK(4)*(-ACTV4*CONST)
DFX(2,5)=-Y(2)*EK(5)*(-ACTV5*CONST)
DFX(3,1)=EK(2)+EK(3)
DFX(3,2)=EK(5)
DFX(3,5)=Y(2)*EK(5)*(-ACTV5*CONST)
DO 65 I=1,5
DO 65 J=1,5
FQ(I,J)=0.
QF(I,J)=0.
QWH(I,J)=0.
QWQ(I,J)=0.
65 CONTINUE
DO 70 I=1,3
DO 70 J=1,5
WH(I,J)=0.
70 CONTINUE
DO 75 K=1,5
DO 75 I=1,3
DO 75 J=1,3
WH(I,K)=WH(I,K)+WF(I,J)*HD(J,K)
75 CONTINUE
DO 80 K=1,5
DO 80 I=1,5
DO 80 J=1,3
QWH(K,I)=QWH(K,I)+QH(K,J)*WH(J,I)
80 CONTINUE
DO 110 K=1,5
DO 110 I=1,5
DO 110 J=1,5
QWQ(K,I)=QWQ(K,I)+QWH(K,J)*Q(J,I)
110 CONTINUE
DO 90 K=1,5
DO 90 I=1,5
DO 90 J=1,5
FQ(K,I)=FQ(K,I)+DFX(K,J)*Q(J,I)
QF(K,I)=QF(K,I)+Q(K,J)*DFX(I,J)
90 CONTINUE

```


C SUBROUTINE FCT ... (CONT'D)

C ESTIMATION OF COVARIANT MATRIX ELEMENT

```
DO 120 I=1,5
DO 120 J=1,5
EQ(I,J)=FQ(I,J)+QF(I,J)-QWQ(I,J)
120 CONTINUE
K=0
DO 130 I=1,5
K=K-I+5
DO 130 J=1,5
IJK=K+I+J
EY(IJK)=EQ(I,J)
130 CONTINUE
DO 140 I=1,NDIM
DERY(I)=EY(I)
140 CONTINUE
141 CONTINUE
RETURN
END
```


C SUBROUTINE RKGM

C SUBROUTINE RKGM

```

C        *****
C        *
C        *                                SUBROUTINE RKGM                                *
C        *                                -----                                        *
C        *
C        *        FUNCTION OF THIS SUBROUTINE                                        *
C        *
C        *                RUNGE-KUTTA-GILL INTEGRATION ROUTINE                        *
C        *
C        *        PARAMETER DEcriptions                                                *
C        *                NDIM.....DIMENSION OF DEPENDENT VARI-                    *
C        *                                                ABLES                                *
C        *                Y(I).....THE DEPENDENT VARIABLES WITH                    *
C        *                                                DIMENSION NDIM                        *
C        *                X.....THE INDEPENDENT VARIABLE                                *
C        *                PRMT(3).....INTEGRATION INTERVAL                                *
C        *                DERY(I).....DERIVATIVE OF STATE FUNCTIONS                        *
C        *
C        *        SUBROUTINE CALLED AND USAGE                                        *
C        *                CALL FCT                                                        *
C        *                CALL OUTP                                                        *
C        *
C        *****

```

SUBROUTINE RKGM

```

      DIMENSION RJ(27),RK(27),RQ(27)
      COMMON X,Y(27),DERY(27),PRMT(3),FREQ(5),EK(5),Q(6,6)
      *,WF(3,3),HD(3,
      *,6),THD(6,3),ZH(3),NDIM,ACTVE(5),ACTV2,ACTV4,ACTV5,L
      *,TEMP
      COMMON RCONC(3)
      H=PRMT(3)
5  RX=X
      DO 10 I=1,NDIM
10  RJ(I)=Y(I)
      CALL FCT
      DO 20 I=1,NDIM
20  RK(I)=H*DERY(I)
      DO 30 I=1,NDIM
      RJ(I)=RJ(I)+0.5*RK(I)
30  RQ(I)=RK(I)
      X=RX+H/2.
      DO 40 I=1,NDIM
40  Y(I)=RJ(I)
      CALL FCT

```


C SUBROUTINE RKGM ... (CONT'D)

```
DO 50 I=1,NDIM
50 RK(I)=H*DERY(I)
SQ=1./SQRT(2.)
DO 60 I=1,NDIM
60 RJ(I)=RJ(I)+(1.-SQ)*(RK(I)-RQ(I))
CA=2.-SQRT(2.)
CB=-2.+3./SQRT(2.)
DO 70 I=1,NDIM
70 RQ(I)=CA*RK(I)+CB*RQ(I)
DO 80 I=1,NDIM
80 Y(I)=RJ(I)
CALL FCT
DO 90 I=1,NDIM
RK(I)=H*DERY(I)
90 RJ(I)=RJ(I)+(1.+SQ)*(RK(I)-RQ(I))
CE=2.+SQRT(2.)
CF=-2.-3./SQRT(2.)
DO 100 I=1,NDIM
100 RQ(I)=CE*RK(I)+CF*RQ(I)
X=RX+H
DO 110 I=1,NDIM
110 Y(I)=RJ(I)
CALL FCT
DO 120 I=1,NDIM
120 RK(I)=H*DERY(I)
DO 130 I=1,NDIM
130 Y(I)=RJ(I)+RK(I)/6.-RQ(I)/3.
CALL OUTP
6 RETURN
END
```


C SUBROUTINE OUTP

C SUBROUTINE OUTP

```

C      ****
C      *
C      *              SUBROUTINE OUTP
C      *              -----
C      *
C      *      PURPOSE
C      *
C      *      THIS SUBROUTINE IS THE OUTPUT ROUTINE TO
C      *      PRINT OUT THE REQUIRED DATA
C      *
C      ****

```

SUBROUTINE OUTP

```

COMMON X,Y(27),DERY(27),PRMT(3),FREQ(5),EK(5),Q(6,6)
*,WF(3,3),HD(3,
*,6),THD(6,3),ZH(3),NDIM,ACTVE(5),ACTV2,ACTV4,ACTV5,L
*,TEMP
COMMON RCONC(3)
GO TO (1,2),L
1 CONTINUE
WRITE(6,5)X,Y(1),Y(2),Y(3),TEMP
5 FORMAT(' ',85X,F5.3,3(2X,F5.4),3X,F5.0)
GO TO 11
2 CONTINUE
9 CONTINUE
ACTVE(4)=ACTV4*Y(4)+ACTV4
ACTVE(5)=ACTV5*Y(5)+ACTV5
WRITE(6,10)X,Y(1),Y(2),Y(3),ACTVE(4),ACTVE(5)
10 FORMAT('+',5X,F5.3,3X,F5.4,3X,F5.4,3X,F5.4,16X,2(3X
*,E13.5))
11 CONTINUE
RETURN
END

```


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